Gaussian operator bases for correlated fermions

J. F. Corney and P. D. Drummond
ARC Centre of Excellence for Quantum-Atom Optics,
University of Queensland, Brisbane 4072, Queensland, Australia.
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We formulate a general multi-mode Gaussian operator basis for fermions, to enable a positive phase-space representation of correlated Fermi states. The Gaussian basis extends existing bosonic phase-space methods to Fermi systems and thus enables first-principles dynamical or equilibrium calculations in quantum many-body Fermi systems. We prove the completeness and positivity of the basis, and derive differential forms for products with one- and two-body operators. Because the basis satisfies fermionic superselection rules, the resulting phase space involves only c-numbers, without requiring anti-commuting Grassmann variables.

I. INTRODUCTION

In this paper we address the issue of how to represent highly correlated fermionic states, for the purposes of efficient calculations in fermionic many-body physics. To this end, we introduce a normally ordered Gaussian operator basis for fermionic density operators. With this basis, earlier phase-space techniques used to represent atomic transitions[1, 2] can be extended to general Fermi systems.

The analogous phase-space methods for bosons were first introduced over a classical phase space[3, 4, 5, 6], which was subsequently extended to a non-classical phase space[7, 8] and then to a complete Gaussian basis [9]. Just as with bosons, the Gaussian basis enables a representation of arbitrary fermionic density operators as a positive distribution over a generalised phase space.

We investigate both number-conserving basis sets, which generalize the usual thermal states used to describe Fermi gases, and non-number-conserving basis sets, which generalize the BCS states found in superconductivity theory[10]. The latter case comprises the most general Gaussian basis.

We concentrate on the foundational issues of the Gaussian representation method, proving three central results:

- the basis is complete,

- the distribution can always be chosen positive,

- all two-body operators map to a second-order differential form.

From these results, it follows that positive-definite Fokker-Planck equations[11] exist for many-body fermionic systems. Such Fokker-Planck equations enable first-principles stochastic numerical simulation methods, either in real time or at finite temperature. They can also be used to obtain novel types of perturbation theory using stochastic diagram techniques[12].

The formulation of the resultant phase-space simulation methods, which, for example, can be applied to the Hubbard model[14], will be given elsewhere[15]. However, we note these methods have similarities to the auxiliary field method[13] used to simplify fermionic path integrals, except that here the Gaussian basis is used to expand the fermionic states themselves, rather than a path integral, which has advantages in terms of giving a greater physical understanding and fewer restrictions in the resulting applications.

To begin, we establish in Sec. II the definition of a Gaussian operator in unnormalised form, and follow this in Sec. III with elementary examples of one- and two-mode Gaussians in order to illustrate the basic structure and the physics underlying it. The two-mode examples include the density operators for thermal and squeezed fermionic states. In Sec. IV, we introduce some notation that is convenient for discussing general Gaussian operators in a multimode system.

The main part of the paper (Section V) introduces the most general class of normalized Gaussian operators and discusses those of its properties that are relevant to its use as a basis set. This section also gives the proofs of the completeness and positivity properties, which are established by expansion in number-state projectors. Other properties are proved by use of Fermi coherent states[16] (Appendix A), and these latter proofs are given in Appendix B.

II. DEFINITIONS

To define Gaussian operators for a given fermionic system, we first decompose it into a set of M orthogonal single-particle modes, or orbitals. With each of these modes, we associate creation and annihilation operators $\widehat{b}_j^\dagger$ and $\widehat{b}_j$, with anticommutation relations

$$
\begin{aligned}
\left[\widehat{b}_j, \widehat{b}_k^\dagger\right]_+ &= \delta_{jk} \\
\left[\widehat{b}_j, \widehat{b}_k\right]_+ &= 0 \ ,
\end{aligned} \tag{2.1}
$$

where $j, k = 1...M$. Thus, $\widehat{\boldsymbol{b}}$ is a column vector of the M annihilation operators, and $\widehat{\boldsymbol{b}}^\dagger$ is a row vector of the corresponding creation operators.

We define a Gaussian operator to be a normally ordered, Gaussian form of annihilation and creation operators. Like a complex number Gaussian, the operator

Gaussian is an exponential of a quadratic form, with the exponential defined by its series representation. We follow the standard convention that fermionic normal ordering includes a sign-change for every operator exchange, so that $:\widehat{b}_k\widehat{b}_j^\dagger := -\widehat{b}_j^\dagger\widehat{b}_k$. Normal ordering is utilized here because it allows us to most directly use Fermi coherent state methods[16] involving Grassmann algebra[17][18], which are described in greater detail in the Appendices. We note that from particle-hole symmetry, it is also possible to obtain an entirely analogous anti-normally ordered representation, which simply exchanges the roles of particles and holes in the formalism.

The most general Gaussian form is a cumbersome object to manipulate, unless products of odd numbers of operators are excluded. Fortunately, restricting the set of Gaussians to those containing only even products can be physically justified on the basis of superselection rules for fermions. Because it is constructed from pairs of operators, this type of Gaussian operator contains no Grassmann variables[16][19].

In order to relate these quadratic expressions to the usual Dirac state-vector notation in the examples that follow, we define number states as:

$$\begin{aligned}
|\vec{n}\rangle &= |n_1\rangle \otimes |n_2\rangle \ldots \otimes |n_M\rangle \\
&= \left(\widehat{b}_1^\dagger\right)^{n_1}\left(\widehat{b}_2^\dagger\right)^{n_2}\ldots\left(\widehat{b}_M^\dagger\right)^{n_M}|0\rangle_M, \quad (2.2)
\end{aligned}$$

where $\vec{n} = (n_1, n_2, \ldots, n_M)$ is a vector of integer occupations and where $|0\rangle_M$ is the M-mode fermion vacuum state.

We also recall some elementary identities which relate quadratic forms in fermion operators to state projection operators. For individual operators, one has the well-known identities:

$$\begin{aligned}
\widehat{b}_j &= |0\rangle_j\langle 1|_j, \\
\widehat{b}_j^\dagger &= |1\rangle_j\langle 0|_j. \quad (2.3)
\end{aligned}$$

Hence, the elementary identities for quadratic products are as follows, for $i < j$:

$$\begin{aligned}
\widehat{b}_i^\dagger\widehat{b}_i &= |1\rangle_i\langle 1|_i\prod_{k\neq i}\hat{1}_k \\
\widehat{b}_i\widehat{b}_i^\dagger &= |0\rangle_i\langle 0|_i\prod_{k\neq i}\hat{1}_k \\
\widehat{b}_i^\dagger\widehat{b}_j &= |1_i, 0_j\rangle\langle 0_i, 1_j|\prod_{k\neq i,j}\hat{1}_k \\
\widehat{b}_j\widehat{b}_i &= |0_i, 0_j\rangle\langle 1_i, 1_j|\prod_{k\neq i,j}\hat{1}_k, \quad (2.4)
\end{aligned}$$

where $\hat{1}_k$ is the identity operator for the $k-$th mode.

Expanding quantum states in terms of an underlying basis set is a widespread procedure in quantum mechanics. However, using the general Gaussian operators in this capacity is nonstandard in several respects. First, one is expanding a quantum density operator over a basis set that includes mixed as well as pure quantum states. Second, the Gaussian operator basis states are not orthogonal. Third, we also allow the basis set to include operators which are not themselves density operators. These additional degrees of freedom prove useful in obtaining the requisite completeness properties. We now give the mathematical form of these basis operators, in unnormalised form; normalized forms $\widehat{\Lambda}_M$, for which $Tr\left(\widehat{\Lambda}_M\right) = 1$, will be introduced in Sec. V.

A. Number-conserving Gaussians

We first consider the special case obtained when the quadratic is of form $\widehat{b}_i^\dagger\widehat{b}_j$, so that it is number-conserving. The most general, number-conserving Gaussian operator can be written as:

$$\begin{aligned}
\widehat{\Lambda}_M^{(u)}(\boldsymbol{\mu}) &= :\exp\left[-\widehat{\boldsymbol{b}}^\dagger\boldsymbol{\mu}\widehat{\boldsymbol{b}}\right]:, \\
&= :\prod_{i,j=1}^M\exp\left[-\widehat{b}_i^\dagger\mu_{ij}\widehat{b}_j\right]: \\
&= :\prod_{i,j=1}^M\left[\hat{1} - \widehat{b}_i^\dagger\mu_{ij}\widehat{b}_j\right]: \quad (2.5)
\end{aligned}$$

where $\boldsymbol{\mu}$ is a complex $M \times M$ matrix. The last result follows because normally ordered products in which the same operator appears more than once are zero, from the anti-commutation relations in Eq. (2.1). For the special case that $\boldsymbol{\mu}$ is a hermitian matrix, the Gaussian operator is just the density operator of a thermal state. If the eigenvalues of $\boldsymbol{\mu}$ are also either 0 or 1, then the Gaussian corresponds to a Slater determinant (i.e. a product of single-mode number states).

It should be noted here that we do not restrict the Gaussian operators of this type to be just thermal states. In general we would wish to consider density matrices that are linear combinations of Gaussian operators, and these can exist as hermitian, positive-definite operators even when composed of Gaussians that have neither property.

B. Non-number-conserving Gaussians

If anomalous products of form $\widehat{b}_i\widehat{b}_j$ are included as well, then the most general non-number-conserving Gaussian is a type of squeezed state:

$$\begin{aligned}
\widehat{\Lambda}_M^{(u)}(\boldsymbol{\mu}, \boldsymbol{\xi}, \boldsymbol{\xi}^+) &= :\exp\left[-\widehat{\boldsymbol{b}}^\dagger\boldsymbol{\mu}\widehat{\boldsymbol{b}} - \frac{1}{2}\left(\widehat{\boldsymbol{b}}\boldsymbol{\xi}^+\widehat{\boldsymbol{b}} + \widehat{\boldsymbol{b}}^\dagger\boldsymbol{\xi}\widehat{\boldsymbol{b}}^\dagger\right)\right]: \\
&= \prod_{i>j}\left[1 - \xi_{ij}\hat{b}_i^\dagger\hat{b}_j^\dagger\right]:\prod_{ij}\left[1 - \mu_{ij}\hat{b}_i^\dagger\hat{b}_j\right]: \times \\
&\quad \times\prod_{i>j}\exp\left[1 - \xi_{ij}^+\hat{b}_i\hat{b}_j\right]. \quad (2.6)
\end{aligned}$$

Here $\boldsymbol{\xi}$, $\boldsymbol{\xi}^+$ are complex antisymmetric $M \times M$ matrices. For the special case that $\boldsymbol{\mu}$ is a hermitian matrix and $\boldsymbol{\xi}^\dagger = \boldsymbol{\xi}^+$, then the Gaussian operator is just the density operator for a squeezed thermal state. Normalized forms $\widehat{\Lambda}_M$, for which $Tr\left(\widehat{\Lambda}_M\right) = 1$, will be introduced later.

As before, we do not restrict the Gaussian operators to be just the squeezed thermal states, even though this represents a large and physically important class of fermionic density operators. By extending the definition to include all exponentials of quadratic forms, we can obtain a more useful set, which is a complete basis with a positive-definite representation for all density operators, as we show in Sec. V.

III. ONE AND TWO MODE GAUSSIAN OPERATORS

In this section we give examples of Gaussian operators in elementary one and two-mode cases. These are sufficient to illustrate the basic identities and ideas. More general results will be given in Sec. V.

A. Single-mode Gaussian operators

An unnormalised Gaussian operator for a single mode has only one possible form:

$$
\begin{aligned}
\widehat{\Lambda}_1^{(u)}(\mu) &= \; : \exp\left[-\mu \widehat{b}^\dagger \widehat{b}\right] : \\
&\equiv \; : \sum_{k=0}^{\infty} \frac{1}{k!}\left(-\mu \widehat{b}^\dagger \widehat{b}\right)^k : ,
\end{aligned} \tag{3.1}
$$

where the exponential is defined, as indicated, by its series representation. Just as in the general case of Eq (2.5), the anticommutivity of the fermionic operators means that only the zeroth and first-order terms in the expansion contribute to the single mode Gaussian, giving the simple result:

$$
\widehat{\Lambda}_1^{(u)}(\mu) \; = \; 1 - \mu \widehat{b}^\dagger \widehat{b}. \tag{3.2}
$$

The normalisation of this Gaussian operator is

$$
\begin{aligned}
N_1 &\equiv \; \text{Tr}\widehat{\Lambda}_1 \\
&= \; 2 - \mu.
\end{aligned} \tag{3.3}
$$

Excluding the point $\mu = 2$, we define the new parameter $n = (1-\mu)/(2-\mu)$, which allows us to write the Gaussian in normalised form as

$$
\begin{aligned}
\widehat{\Lambda}_1(n) &= \; (1-n) : \exp\left[-\left(2 + 1/(n-1)\right)\widehat{b}^\dagger \widehat{b}\right] : \\
&= \; (1-n)\widehat{b}\widehat{b}^\dagger + n\widehat{b}^\dagger \widehat{b} \\
&= \; (1-n)\left|0\right\rangle\left\langle 0\right| + n\left|1\right\rangle\left\langle 1\right|.
\end{aligned} \tag{3.4}
$$

If n is real, then Eq(3.4) shows directly that $\widehat{\Lambda}_1(n)$ is the density operator corresponding to a mixture of number states in the one-mode case. The expectation value of the fermion occupation $\widehat{n} \equiv \widehat{b}^\dagger \widehat{b}$ is just the variable n.

1. Completeness and positivity

As two special cases we obtain the number states:

$$
\begin{aligned}
\left|0\right\rangle\left\langle 0\right| &= \; \widehat{\Lambda}_1(0) \\
\left|1\right\rangle\left\langle 1\right| &= \; \widehat{\Lambda}_1(1),
\end{aligned} \tag{3.5}
$$

which implies that just these two single-mode Gaussians form a complete basis set for a number-conserving subset of Hilbert space. Because super-selection rules prohibit superpositions of states differing by odd numbers of fermions, this is the most general case possible. Furthermore, we see from Eq (3.5) that the most general single-mode density matrix can be expanded as a mixture of Gaussians with *positive* coefficients, since $0 \leq n \leq 1$:

$$
\widehat{\rho} = (1-n)\widehat{\Lambda}_1(0) + n\widehat{\Lambda}_1(1) . \tag{3.6}
$$

Additionally in the one-mode case, all physical density operators are also Gaussian operators $\widehat{\rho} = \widehat{\Lambda}_1(n)$, which is another proof of positivity and completeness.

It is clear from these examples that the Gaussian operators are *overcomplete*: a physical density matrix may be represented by more than one positive distribution over the Gaussians. The most general single-mode Gaussian operator, with n complex, provides an even larger over-complete basis for physical density matrices, even though such Gaussians are not always physical density matrices themselves. For example, any uniform-phase distribution over Gaussian states gives the zero-particle state:

$$
\left|0\right\rangle\left\langle 0\right| \; = \; \int d\phi \widehat{\Lambda}_1(re^{i\phi}). \tag{3.7}
$$

From the usual hole-particle symmetry of fermion states, the single-particle state is similarly obtained from:

$$
\left|1\right\rangle\left\langle 1\right| \; = \; \int d\phi \widehat{\Lambda}_1(1 - re^{i\phi}). \tag{3.8}
$$

B. Two-mode number-conserving Gaussian operators

A straightforward extension of the generalized thermal Gaussian form to two modes gives

$$
\begin{aligned}
\widehat{\Lambda}_2^{(u)}(\boldsymbol{\mu}) &= \; : \exp\left[-\sum_{i,j=1}^{2} \mu_{ij}\widehat{b}_i^\dagger \widehat{b}_j\right] : \\
&= \; 1 - \sum_{i,j=1}^{2} \mu_{ij}\widehat{b}_i^\dagger \widehat{b}_j + \det\boldsymbol{\mu}\,\widehat{b}_1^\dagger \widehat{b}_2^\dagger \widehat{b}_2 \widehat{b}_1,
\end{aligned} \tag{3.9}
$$

where the μ_{ij} are the elements of the 2×2 matrix $\boldsymbol{\mu}$. The last step follows by explicitly expanding the general result in Eq (2.5), while taking account of the sign changes during normal ordering. Again, the series expansion contains all possible normally ordered nonzero products of the $\widehat{b}_i^\dagger \widehat{b}_j$ pairs. In terms of two-mode number-state projectors, the Gaussian operator is

$$
\begin{aligned}
\widehat{\Lambda}_2^{(u)}(\boldsymbol{\mu}) \;=\; & |00\rangle \langle 00| + (1 - \mu_{11}) |10\rangle \langle 10| \\
& + (1 - \mu_{22}) |01\rangle \langle 01| \\
& + (1 - \mu_{11} - \mu_{22} + \det \boldsymbol{\mu}) |11\rangle \langle 11| \\
& - \mu_{12} |10\rangle \langle 01| - \mu_{21} |01\rangle \langle 10| . \quad (3.10)
\end{aligned}
$$

1. Normalisation and Moments

Following from Eq. (3.10), the normalisation is

$$
N_2 \;=\; 4 - 2\mu_{11} - 2\mu_{22} + \det \boldsymbol{\mu}. \quad (3.11)
$$

Defining the matrix $\boldsymbol{n} = \mathbf{I} - (2\mathbf{I} - \boldsymbol{\mu}^T)^{-1}$, where $\mathbf{I}$ is the 2×2 identity matrix, we can write the normalised two-mode Gaussian as

$$
\begin{aligned}
\widehat{\Lambda}_2(\mathbf{n}) \;=\; & \det [\mathbf{I} - \mathbf{n}] : \exp \left[-\widehat{\boldsymbol{b}}^\dagger \left(2\mathbf{I} + [\mathbf{n}^T - \mathbf{I}]^{-1} \right) \widehat{\boldsymbol{b}} \right] : \\
\;=\; & \det [\mathbf{I} - \mathbf{n}] |00\rangle \langle 00| \\
& + (n_{11}(1 - n_{22}) + n_{12}n_{21}) |10\rangle \langle 10| \\
& + (n_{22}(1 - n_{11}) + n_{12}n_{21}) |01\rangle \langle 01| \\
& + \det \mathbf{n} |11\rangle \langle 11| + n_{21} |10\rangle \langle 01| + n_{12} |01\rangle \langle 10| .
\end{aligned}
$$

(3.12)

If $\mathbf{n}$ is an Hermitian matrix, then the two-mode Gaussian corresponds to the density matrix of a mixture of states of different total number, with coherences $n_{12} = n_{21}^*$ between states of the same total number.

Normally ordered first-order correlations of the Gaussian density matrices correspond to elements of $\mathbf{n}$:

$$
\left\langle \widehat{b}_i^\dagger \widehat{b}_j \right\rangle_{\widehat{\Lambda}} \;\equiv\; \mathrm{Tr} \widehat{b}_i^\dagger \widehat{b}_j \widehat{\Lambda}_2 = n_{ij}, \quad (3.13)
$$

and higher-order correlations reduce to products of first-order averages, for example,

$$
\left\langle \widehat{b}_1^\dagger \widehat{b}_1 \widehat{b}_2^\dagger \widehat{b}_2 \right\rangle_{\widehat{\Lambda}} \;=\; n_{11}n_{22} - n_{12}n_{21}. \quad (3.14)
$$

This kind of factorisation of higher-order correlations could be taken as the defining characteristic of a Gaussian state, and more generally, Gaussian operators, rather than the more formal operator definition given by Eq. (3.9). In other words, Gaussian operators have both a Gaussian form and generate Gaussian statistics. The connection between these two defining features can be made more explicit by use of a moment-generating function, or characteristic function, which is considered in Appendix B.

Because the matrix $\mathbf{n}$ is Hermitian for a Gaussian that is a density operator, it can be diagonalised, corresponding to a change of single-particle basis. In this diagonalised basis, since the coherences are zero, the density operator is a mixture of number states, totally characterised by average occupation numbers. In other words, these Gaussian operators correspond to two-mode thermal states.

2. Completeness

We wish to show first that any number-conserving two-mode density matrix can be expanded in terms of Gaussian operators, and second that this can be done with positive expansion coefficients. The first result follows if we can represent all the number-state projectors between states of the same total number using Gaussian operators. By inspection of Eq (3.12) above, we find that:

$$
\begin{aligned}
|00\rangle \langle 00| \;=\; & \widehat{\Lambda}_2(\mathbf{0}) \\
|10\rangle \langle 10| \;=\; & \widehat{\Lambda}_2 \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right) \\
|01\rangle \langle 01| \;=\; & \widehat{\Lambda}_2 \left(\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right) \\
|11\rangle \langle 11| \;=\; & \widehat{\Lambda}_2(\mathbf{I}) \\
n_{21} |10\rangle \langle 01| \;=\; & \widehat{\Lambda}_2 \left(\begin{pmatrix} n_1 & 0 \\ n_{21} & n_2 \end{pmatrix} \right) - \widehat{\Lambda}_2 \left(\begin{pmatrix} n_1 & 0 \\ 0 & n_2 \end{pmatrix} \right) \\
n_{12} |01\rangle \langle 10| \;=\; & \widehat{\Lambda}_2 \left(\begin{pmatrix} n_1 & n_{12} \\ 0 & n_2 \end{pmatrix} \right) - \widehat{\Lambda}_2 \left(\begin{pmatrix} n_1 & 0 \\ 0 & n_2 \end{pmatrix} \right)
\end{aligned}
$$

(3.15)

Thus, the two-mode Gaussians form a complete operator basis for all number-conserving density matrices.

3. Positivity

Not only is the two-mode Gaussian a complete representation, but it is also a positive one: any two-mode number-conserving density operator can be written as a positive distribution over Gaussian operators. To see this, note that while the expression for the projection operators, Eq (3.15), includes terms with negative coefficients, the projectors involved are the off-diagonal ones. Since density matrices are positive-definite, off-diagonal projectors can only occur in combination with diagonal projectors. We take this into account in what follows.

Any two-mode density operator can be expanded into number-state projector operators as follows:

$$
\widehat{\rho} \;=\; \sum_{\vec{n}} \sum_{\vec{n}'} \rho_{\vec{n}, \vec{n}'} |\vec{n}\rangle \langle \vec{n}'| , \quad (3.16)
$$

where $\vec{n}$ and $\vec{n}'$ are vectors of integer occupation numbers: $\vec{n} = (n_1, n_2)$, $\vec{n}' = (n_1', n_2')$. Here $\rho_{\vec{n}, \vec{n}'} = 0$ if $\sum_j n_j \neq$

$\sum_j n'_j$, because of total-number conservation. Using the relations in Eq. (3.15), we can write the density operator as

$$\widehat{\rho} = \sum_{\vec{n}} \frac{1}{2}\rho_{\vec{n},\vec{n}} \left[\widehat{\Lambda}_2(\begin{pmatrix} n_1 & 2\rho_{(01),(10)} \\ 0 & n_2 \end{pmatrix})) \right.$$
$$\left. + \widehat{\Lambda}_2(\begin{pmatrix} n_1 & 0 \\ 2\rho_{(10),(01)} & n_2 \end{pmatrix})) \right]. \quad (3.17)$$

Since the diagonal coefficients $\rho_{\vec{n},\vec{n}}$ are positive and sum to one, the Gaussian operators form the basis of a probabilistic representation of any two-mode density operator.

While any two-mode number-conserving density matrix can be expanded in the form in Eq. (3.17), there are often more direct representations. For example, as Eq. (3.20) below shows, the entangled state $|\phi\rangle = \alpha|10\rangle + \beta|01\rangle$ can be represented by just one term, rather than the four terms that result from Eq. (3.17).

4. Correlation and entanglement

We first note that any uncorrelated product of number state mixtures can be represented exactly:

$$\widehat{\rho}_{n_1} \otimes \widehat{\rho}_{n_2} \equiv \{(1-n_1)|0\rangle\langle 0| + n_1|1\rangle\langle 1|\}$$
$$\otimes \{(1-n_2)|0\rangle\langle 0| + n_2|1\rangle\langle 1|\}$$
$$= \widehat{\Lambda}_2(\begin{pmatrix} n_1 & 0 \\ 0 & n_2 \end{pmatrix}). \quad (3.18)$$

As well as these uncorrelated mixtures, the Gaussian basis can also be used to represent a mixture with correlations between the modes, this time as a sum (with positive weights) of two terms:

$$A|00\rangle\langle 00| + B|11\rangle\langle 11| = A\widehat{\Lambda}_2(\mathbf{0}) + B\widehat{\Lambda}_2(\mathbf{I}). \quad (3.19)$$

Importantly, superpositions of number states, corresponding to entangled states, can also be represented, subject to total-number conservation. For example, the density matrix corresponding to the state $|\phi\rangle = \alpha|10\rangle + \beta|01\rangle$ is

$$|\phi\rangle\langle\phi| = |\alpha|^2|10\rangle\langle 10| + \alpha\beta^*|10\rangle\langle 01|$$
$$+\alpha^*\beta|01\rangle\langle 10| + |\beta|^2|01\rangle\langle 01|$$
$$= \widehat{\Lambda}_2(\begin{pmatrix} |\alpha|^2 & \alpha^*\beta \\ \alpha\beta^* & |\beta|^2 \end{pmatrix}). \quad (3.20)$$

Thus the number-conserving Gaussian operators even include entangled density matrices, making them a powerful tool for representing highly correlated states.

This property of being able to represent such Bell-like entangled states with the hermitian subset of Gaussian operators, is different to the case of Gaussian expansions for bosons. A typical example of this type of nonclassical representation is the positive P-representation[7, 8], which must use a non-hermitian basis to obtain a positive distribution that can represent all two-mode density matrices, such as those that violate a Bell inequality[20].

C. Two-mode squeezed Gaussian operators

Equation (3.9) does not represent the most general two-mode Gaussian form, as the quadratic form does not yet include terms such as $\widehat{b}_1\widehat{b}_2$. Incorporating such anomalous products, we can write the most general Gaussian operator in normalised form as:

$$\widehat{\Lambda}_2^{(u)}(\boldsymbol{\mu},\xi,\xi^+) = :\exp\left[-\sum_{i,j=1}^{2}\mu_{ij}\widehat{b}_i^\dagger\widehat{b}_j - \xi^+\widehat{b}_1\widehat{b}_2 - \xi\widehat{b}_2^\dagger\widehat{b}_1^\dagger\right]:$$
$$= 1 - \sum_{i,j=1}^{2}\mu_{ij}\widehat{b}_i^\dagger\widehat{b}_j - \xi\widehat{b}_2^\dagger\widehat{b}_1^\dagger - \xi^+\widehat{b}_1\widehat{b}_2$$
$$+ \left(\det\boldsymbol{\mu} + \xi\xi^+\right)\widehat{b}_1^\dagger\widehat{b}_2^\dagger\widehat{b}_2\widehat{b}_1, \quad (3.21)$$

where ξ and ξ^+ are independent complex numbers. The two additional operator terms in the expansion, $\widehat{b}_2^\dagger\widehat{b}_1^\dagger$ and $\widehat{b}_1\widehat{b}_2$, are projectors between states of different total number:

$$\widehat{b}_1\widehat{b}_2 = -|00\rangle\langle 11|,$$
$$\widehat{b}_2^\dagger\widehat{b}_1^\dagger = -|11\rangle\langle 00|, \quad (3.22)$$

which are the kinds of coherences that appear in the density matrices of two-mode squeezed states.

1. Normalisation and Moments

The normalisation of the squeezed Gaussian is

$$N_2 = 4 - 2\mu_{11} - 2\mu_{22} + \det\boldsymbol{\mu} + \xi\xi^+. \quad (3.23)$$

To incorporate this into a normalised Gaussian, we redefine the $\mathbf{n}$ matrix to be

$$\mathbf{n} = \mathbf{I} - \frac{N_2}{N_2 - \xi\xi^+}\left(2\mathbf{I} - \boldsymbol{\mu}^T\right)^{-1}, \quad (3.24)$$

and introduce rescaled squeezing parameters $m = -\xi/N_2$, $m^+ = -\xi^+/N_2$. The normalised form is then

$$\widehat{\Lambda}_2(\mathbf{n}, m, m^+) = \left(\det[\mathbf{I} - \mathbf{n}] + mm^+\right) \times$$
$$:\exp\left[\left(\widehat{\boldsymbol{b}}^\dagger\widehat{\boldsymbol{b}}^T\right)\left(\underline{I} - \underline{\sigma}^{-1}/2\right)\begin{pmatrix} \widehat{\boldsymbol{b}} \\ \widehat{\boldsymbol{b}}^{\dagger T} \end{pmatrix}\right]:, \quad (3.25)$$

where the 4×4 matrices $\underline{I}$ and $\underline{\sigma}$ are defined to be

$$\underline{I} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\underline{\sigma} = \begin{bmatrix} n_{11}-1 & n_{21} & 0 & m \\ n_{12} & n_{22}-1 & -m & 0 \\ 0 & -m^+ & 1-n_{11} & -n_{12} \\ m^+ & 0 & -n_{21} & 1-n_{22} \end{bmatrix}. \quad (3.26)$$

In terms of number-state projectors, the normalised Gaussian is a generalisation of the number-conserving case, but with the additional non-number-conserving projectors:

$$
\begin{aligned}
\widehat{\Lambda}_2(\underline{\sigma}) &= \left(\det\left[\mathbf{I} - \mathbf{n}\right] + mm^+\right) |00\rangle\langle00| \\
&\quad + \left(n_{11}(1 - n_{22}) + n_{12}n_{21} - mm^+\right) |10\rangle\langle10| \\
&\quad + \left(n_{22}(1 - n_{11}) + n_{12}n_{21} - mm^+\right) |01\rangle\langle01| \\
&\quad + \left(\det \mathbf{n} + mm^+\right) |11\rangle\langle11| \\
&\quad + n_{21} |10\rangle\langle01| + n_{12} |01\rangle\langle10| \\
&\quad - m |11\rangle\langle00| - m^+ |00\rangle\langle11| .
\end{aligned} \tag{3.27}
$$

In addition to the normal fluctuations of Eq. (3.13), the squeezed Gaussians also contain anomalous fluctuations, which are just equal to the new variables m and m^+:

$$
\begin{aligned}
\left\langle \widehat{b}_1 \widehat{b}_2 \right\rangle_{\widehat{\Lambda}} &= m, \\
\left\langle \widehat{b}_2^\dagger \widehat{b}_1^\dagger \right\rangle_{\widehat{\Lambda}} &= m^+,
\end{aligned} \tag{3.28}
$$

which implies that for $\widehat{\Lambda}_2(\mathbf{n}, m, m^+)$ to be a density matrix, m and m^+ must be complex-conjugate. The second-order correlation generalises to

$$
\left\langle \widehat{b}_1^\dagger \widehat{b}_1 \widehat{b}_2^\dagger \widehat{b}_2 \right\rangle_{\widehat{\Lambda}} = n_{11}n_{22} - n_{12}n_{21} + mm^+, \tag{3.29}
$$

which again corresponds to the decorrelation that occurs in a state with Gaussian statistics.

2. Completeness

From Eq. (3.27), it follows that the squeezed Gaussians provide a complete two-mode fermionic basis, not only for the number conserving subspace, but also for all states containing superpositions of states whose difference in total number is even. To see this, note that the projectors between number the $|00\rangle$ and $|11\rangle$ number states can be written explicitly in terms of the Gaussian operators as

$$
\begin{aligned}
m |11\rangle\langle00| &= \widehat{\Lambda}_2(\mathbf{n}, -m, 0) - \widehat{\Lambda}_2(\mathbf{n}, 0, 0), \\
m^+ |00\rangle\langle11| &= \widehat{\Lambda}_2(\mathbf{n}, 0, -m^+) - \widehat{\Lambda}_2(\mathbf{n}, 0, 0),
\end{aligned} \tag{3.30}
$$

for any $\mathbf{n}$. These projectors, together with those of Eq. (3.15), span the complete Hilbert space of density matrices in question.

3. Positivity

Just as for the number-conserving case, we can write any physical density operator as a positive distribution over Gaussian operators:

$$
\begin{aligned}
\widehat{\rho} &= \sum_{\vec{n}} \sum_{\vec{n}'} \rho_{\vec{n},\vec{n}'} |\vec{n}\rangle\langle\vec{n}'| \\
&= \sum_{\vec{n}} \frac{1}{2} \rho_{\vec{n},\vec{n}} \\
&\quad \times \left[\widehat{\Lambda}_2\!\left(\begin{pmatrix} n_1 & 2\rho_{(01),(10)} \\ 0 & n_2 \end{pmatrix}, -2\rho_{(11,00)}, 0 \right) \right. \\
&\quad \left. + \widehat{\Lambda}_2\!\left(\begin{pmatrix} n_1 & 0 \\ 2\rho_{(10),(01)} & n_2 \end{pmatrix}, 0, -2\rho_{(00,11)} \right) \right]
\end{aligned} \tag{3.31}
$$

Thus the Gaussians form the basis of a probabilistic representation of any physical two-mode density operator. The ability to represent physical density matrices with the Gaussian basis, either as a single element or by a positive distribution over basis elements, is important for calculating dynamical simulations of quantum systems via probabilistic methods.

4. Entanglement

Again, these types of Gaussians can directly correspond to entangled density matrices, without having to consider expansions over several elements. But now superpositions of different total number can be represented. As an example of these additional kinds of physical states that the squeezed Gaussians can represent, consider the entangled non-number-conserving superposition state: $|\psi\rangle = \left[|00\rangle + |11\rangle\right]/\sqrt{2}$. This can be represented by a single Gaussian:

$$
\begin{aligned}
|\psi\rangle\langle\psi| &= \frac{1}{2}\left[|00\rangle\langle00| + |00\rangle\langle11| + |11\rangle\langle00| + |11\rangle\langle11|\right] \\
&= \widehat{\Lambda}_2(\tfrac{1}{2}\mathbf{I}, -\tfrac{1}{2}, -\tfrac{1}{2}).
\end{aligned} \tag{3.32}
$$

Hence, the more general type of Gaussian basis element considered here is considerably more powerful for representing entangled and correlated states than the number-conserving basis set.

IV. MULTIMODE DECOMPOSITION OF FERMI SYSTEMS

So far we have considered only one- and two-mode systems, to illustrate the basic physical properties of Gaussian operators. As we saw, the Gaussian operators could easily be written in terms of number-state projectors. The power of the Gaussian operators as a basis in its own right becomes apparent for multimode systems, for which the number-state basis becomes unusable.

Before defining the general Gaussian basis for a system with many degrees of freedom, we define some mathematical notation and conventions that will be of subsequent use. As before, we define $\widehat{\boldsymbol{b}}$ as a column vector of the M

annihilation operators, and $\widehat{\boldsymbol{b}}^\dagger$ as a row vector of the corresponding creation operators. We also introduce an extended column vector of all $2M$ operators: $\underline{\widehat{b}} = (\widehat{\boldsymbol{b}}^T, \widehat{\boldsymbol{b}}^\dagger)^T$, with an adjoint row vector defined as $\underline{\widehat{b}}^\dagger = (\widehat{\boldsymbol{b}}^\dagger, \widehat{\boldsymbol{b}}^T)$. Writing these out in full, we get:

$$\underline{\widehat{b}} = \begin{pmatrix} \widehat{b}_1 \\ \vdots \\ \widehat{b}_M \\ \widehat{b}_1^\dagger \\ \vdots \\ \widehat{b}_M^\dagger \end{pmatrix}, \quad \underline{\widehat{b}}^\dagger = \left(\widehat{b}_1^\dagger, ..., \widehat{b}_M^\dagger, \widehat{b}_1, ..., \widehat{b}_M \right) . \quad (4.1)$$

Throughout the paper, we print length-M vectors and $M \times M$ matrices in bold type, and index them where necessary with Latin indices: $j = 1, ..., M$. Length-$2M$ vectors we denote with an underline and $2M \times 2M$ matrices we denote with a double underline. These extended vectors and matrices are indexed where necessary with Greek indices: $\mu = 1, ..., 2M$. Note that an object such as $\underline{\widehat{b}}\,\underline{\widehat{b}}^\dagger$ is a $2M \times 2M$ matrix:

$$\widetilde{\underline{\widehat{b}}\,\underline{\widehat{b}}^\dagger} = \begin{bmatrix} \widehat{\mathbf{b}}\widehat{\mathbf{b}}^\dagger & \widehat{\mathbf{b}}\widehat{\mathbf{b}}^T \\ \widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^\dagger & \widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^T \end{bmatrix} , \quad (4.2)$$

whereas $\underline{\widehat{b}}^\dagger \underline{\widehat{b}} = \sum_k \widehat{b}_k^\dagger \widehat{b}_k + \widehat{b}_k \widehat{b}_k^\dagger (= M)$ is a scalar. More general kinds of vectors are denoted with an arrow notation: $\overrightarrow{\mu}$.

For products of operators, we make use of normal and antinormal ordering concepts. Normal ordering, denoted by $: \cdots :$, is defined as in the bosonic case, with all annihilation operators to the right of the creation operators, except that each pairwise reordering involved induces a sign change, e. g. : $\widehat{b}_i \widehat{b}_j^\dagger := -\widehat{b}_j^\dagger \widehat{b}_i$. The sign changes are necessary so that the anticommuting natures of the Fermi operators can be accommodated without ambiguity. We define *anti*normal ordering similarly, and denote it via curly braces: $\{\widehat{b}_j^\dagger \widehat{b}_i\} = -\widehat{b}_i \widehat{b}_j^\dagger$. More generally, we can define nested orderings, in which the outer ordering does not reorder the inner one. For example, $\{: \widehat{O}\widehat{b}_j^\dagger : \widehat{b}_i\} = -\widehat{b}_i \widehat{b}_j^\dagger : \widehat{O} :$, where $\widehat{O}$ is some operator.

For example, the different orderings of pairs are, in block matrix form,

$$: \widehat{b}_\mu \widehat{b}_\nu^\dagger := -: \widehat{b}_\nu^\dagger \widehat{b}_\mu : = \begin{bmatrix} -\widehat{b}_j^\dagger \widehat{b}_i & \widehat{b}_i \widehat{b}_j \\ \widehat{b}_i^\dagger \widehat{b}_j^\dagger & \widehat{b}_i^\dagger \widehat{b}_j \end{bmatrix} ,$$

$$\left\{ \widehat{b}_\mu \widehat{b}_\nu^\dagger \right\} = -\left\{ \widehat{b}_\nu^\dagger \widehat{b}_\mu \right\} = \begin{bmatrix} \widehat{b}_i \widehat{b}_j^\dagger & \widehat{b}_i \widehat{b}_j \\ \widehat{b}_i^\dagger \widehat{b}_j^\dagger & -\widehat{b}_j \widehat{b}_i^\dagger \end{bmatrix} . \quad (4.3)$$

Note that this convention means that the relation between the two orderings is

$$: \underline{\widehat{b}}\,\underline{\widehat{b}}^\dagger : = \underline{\underline{I}} + \left\{ \underline{\widehat{b}}\,\underline{\widehat{b}}^\dagger \right\} , \quad (4.4)$$

where $\underline{\underline{I}}$ is the constant matrix

$$\underline{\underline{I}} \equiv \begin{bmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} , \quad (4.5)$$

in which $\mathbf{0}$ and $\mathbf{I}$ are the $M \times M$ zero and identity matrices, respectively.

When ordering products that contain a Gaussian operator $\widehat{\Lambda}$ (and later the density operator), we do not change the ordering of $\widehat{\Lambda}$ itself; the other operators are merely reordered around it. Thus $\left\{ : \widehat{\Lambda}\,\widehat{b}_i^\dagger : \widehat{b}_j \right\} = -\widehat{b}_j\,\widehat{b}_i^\dagger \widehat{\Lambda}$. The different possible quadratic orderings containing a Gaussian operator can thus be written in matrix form as

$$: \underline{\widehat{b}}\,\underline{\widehat{b}}^\dagger \widehat{\Lambda} : = \begin{bmatrix} -\left(\widehat{\boldsymbol{b}}^{\dagger T}\widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^T \right)^T & \widetilde{\widehat{\Lambda}\widehat{\boldsymbol{b}}\widehat{\boldsymbol{b}}^T} \\ \widehat{\boldsymbol{b}}^{\dagger T}\widehat{\boldsymbol{b}}^\dagger \widehat{\Lambda} & \widehat{\boldsymbol{b}}^{\dagger T}\widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^T \end{bmatrix} ,$$

$$\left\{ \underline{\widehat{b}}\,\underline{\widehat{b}}^\dagger \widehat{\Lambda} \right\} = \begin{bmatrix} \widehat{\boldsymbol{b}}\widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^\dagger & \widehat{\boldsymbol{b}}\widehat{\boldsymbol{b}}^T \widehat{\Lambda} \\ \widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^{\dagger T}\widehat{\boldsymbol{b}}^\dagger & -\left(\widehat{\boldsymbol{b}}\widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^\dagger \right)^T \end{bmatrix} ,$$

$$\left\{ \underline{\widehat{b}} : \underline{\widehat{b}}^\dagger \widehat{\Lambda} : \right\} = \begin{bmatrix} \widehat{\boldsymbol{b}}\widehat{\boldsymbol{b}}^\dagger \widehat{\Lambda} & \widehat{\boldsymbol{b}}\widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^T \\ -\left(\widehat{\boldsymbol{b}}^{\dagger T}\widehat{\Lambda}\widehat{\boldsymbol{b}}^\dagger \right)^T & -\left(\widetilde{\widehat{\Lambda}\widehat{\boldsymbol{b}}\widehat{\boldsymbol{b}}^\dagger} \right)^T \end{bmatrix} ,$$

$$\left\{ : \widehat{\Lambda}\underline{\widehat{b}} : \underline{\widehat{b}}^\dagger \right\} = \begin{bmatrix} \widetilde{\widehat{\Lambda}\widehat{\boldsymbol{b}}\widehat{\boldsymbol{b}}^\dagger} & -\left(\widehat{\boldsymbol{b}}\widetilde{\widehat{\Lambda}}\widehat{\boldsymbol{b}}^T \right)^T \\ \widehat{\boldsymbol{b}}^{\dagger T}\widehat{\Lambda}\widehat{\boldsymbol{b}}^\dagger & -\left(\widehat{\boldsymbol{b}}\widehat{\boldsymbol{b}}^\dagger \widehat{\Lambda} \right)^T \end{bmatrix} . \quad (4.6)$$

V. NORMALIZED GAUSSIAN OPERATORS

A. Definition

We define a normalized Gaussian operator $\widehat{\Lambda}$ to be the most general Gaussian form of fermionic annihilation and creation operators, with zero displacement and unit trace. Using the extended-vector notation, we first write the normally-ordered Gaussian in an unnormalized form as

$$\widehat{\Lambda}^{(u)}(\boldsymbol{\mu}, \boldsymbol{\xi}, \boldsymbol{\xi}^+) = : \exp\left[\underline{\widehat{b}}^\dagger \left(\underline{\underline{I}} - \underline{\underline{\sigma}}^{-1}/2 \right) \underline{\widehat{b}} \right] : , \quad (5.1)$$

where we have introduced a new extended $2M \times 2M$ covariance matrix $\underline{\underline{\sigma}}$ defined in terms of $\boldsymbol{\mu}, \boldsymbol{\xi}, \boldsymbol{\xi}^+$ so that:

$$\underline{\underline{\sigma}}^{-1} = 2\underline{\underline{I}} + \begin{bmatrix} \boldsymbol{\mu} & \boldsymbol{\xi} \\ \boldsymbol{\xi}^+ & -\boldsymbol{\mu}^T \end{bmatrix} . \quad (5.2)$$

The introduction of the generalized covariance $\underline{\underline{\sigma}}$ allows the matrix to be written in a normalised form, using the results of Appendix B, together with an explicit complex amplitude factor Ω:

$$\widehat{\Lambda}(\overrightarrow{\lambda}) \;=\; \Omega \mathrm{Pf}\left[\underline{\underline{\sigma_A}}\right] : \exp\left[\widehat{\underline{b}}^{\dagger}\left(\underline{I} - \underline{\underline{\sigma}}^{-1}/2\right)\widehat{\underline{b}}\right] : \;.$$
(5.3)

The normalisation is one obvious difference with the conventional complex-number or bosonic Gaussian forms[9]. Chosen to ensure that $\mathrm{Tr}\,\widehat{\Lambda} = \Omega$, it contains the Pfaffian of an antisymmetric form $\underline{\underline{\sigma_A}}$ of the covariance. The choice of anti-symmetrisation is given in Appendix B; other choices will lead, in general, to additional sign factors. Now the square of the Pfaffian of an antisymmetric matrix is equal to its determinant, and the determinant of $\underline{\underline{\sigma_A}}$ differs from that of $\underline{\underline{\sigma}}$ by a constant sign (see Appendix B). Thus $|\mathrm{Pf}\left[\underline{\underline{\sigma_A}}\right]| = |\sqrt{\det\left[\underline{\underline{\sigma}}\right]}|$, and as we shall see, the relative phase between the two does not appear in later identities. The additional variable Ω plays the role of a weighting factor in the expansion that allows us to represent unnormalised density operators and to introduce 'stochastic gauges' in the drift[21, 22].

The covariance has a type of generalized Hermitian antisymmetry, which can be written as $\underline{\underline{\sigma}} = -\underline{\underline{\sigma}}^{+}$, with the definition that:

$$\begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{bmatrix}^{+} \equiv \begin{bmatrix} \mathbf{d} & \mathbf{c} \\ \mathbf{b} & \mathbf{a} \end{bmatrix}^{T} .$$
(5.4)

It is this generalised antisymmetry that allows the covariance to be transformed into an explicitly antisymmetric matrix. The covariance can also be broken down into the physically significant $M \times M$ submatrices $\mathbf{n}$, $\mathbf{m}$ and $\mathbf{m}^{+}$:

$$\underline{\underline{\sigma}} \;=\; \begin{bmatrix} \mathbf{n^T} - \mathbf{I} & \mathbf{m} \\ \mathbf{m}^{+} & \mathbf{I} - \mathbf{n} \end{bmatrix} ,$$
(5.5)

Here $\mathbf{n}$ is a complex matrix, which corresponds to the normal Green's function in many-body terminology, while $\mathbf{m}$ and $\mathbf{m}^{+}$ are two independent antisymmetric complex matrices that correspond to anomalous Green's functions, as we will show in the next section.

Thus the total parametrization of a general Gaussian operator is

$$\overrightarrow{\lambda} = (\Omega, \mathbf{n}, \mathbf{m}, \mathbf{m}^{+}) ,$$
(5.6)

consisting of $1 + p = 1 + M(2M - 1)$ parameters in all. However, for many systems, only a subset of all Gaussian operators is required for a complete representation of the density operator. One important subset is the set of generalised thermal states, for which $\mathbf{m} = \mathbf{m}^{+} = \mathbf{0}$. In this case, from Appendix B, and using the result that $[2\mathbf{I}-\boldsymbol{\mu}] = [\mathbf{I}-\mathbf{n}]^{-1}$, the normalization factor is $\det[\mathbf{I} - \mathbf{n}]$. The normalized thermal Gaussians therefore can be written:

$$\widehat{\Lambda}(\overrightarrow{\lambda}) \;=\; \Omega \det[\mathbf{I} - \mathbf{n}] : \exp\left[-\widehat{\mathbf{b}}^{\dagger}\left(2\mathbf{I} + \left(\mathbf{n}^{T} - \mathbf{I}\right)^{-1}\right)\widehat{\mathbf{b}}\right] : \;.$$
(5.7)

In order to use the Gaussian operator basis, we need to make use of a number of basic results. The proof of many of these can be established, as we show in Appendix B, with Fermi coherent states and Grassmann algebra, the basics of which are given in Appendix A. However the final results do not contain any Grassmann variables.

B. Trace Properties

Some basic traces are

$$\mathrm{Tr}\left[\widehat{\Lambda}\right] \;=\; \Omega ,$$
$$\mathrm{Tr}\left[\underline{b}\,\widehat{\Lambda}\right] \;=\; 0 ,$$
$$\mathrm{Tr}\left[: \widehat{\underline{b}}\,\widehat{\underline{b}}^{\dagger}\,\widehat{\Lambda} : \right] \;=\; \Omega\underline{\underline{\sigma}} .$$
(5.8)

The first of these is the normalisation, proved as theorem 1 in Appendix B. That the second is zero follows from the fact that the Gaussians are constructed from pairs of ladder operators and thus cannot correspond to a superposition of states whose total fermion numbers differ by one. The same result holds for the trace with any odd product. The third trace, proved as theorem 2 in Appendix B, allows us to calculate first-order moments. In terms of the $M \times M$ submatrices, these become:

$$\mathrm{Tr}\left[\widehat{b}_i^{\dagger}\widehat{b}_j\,\widehat{\Lambda}\right] \;=\; \Omega n_{ij} ,$$
$$\mathrm{Tr}\left[\widehat{b}_i\widehat{b}_j\,\widehat{\Lambda}\right] \;=\; \Omega m_{ij} ,$$
$$\mathrm{Tr}\left[\widehat{b}_i^{\dagger}\widehat{b}_j^{\dagger}\,\widehat{\Lambda}\right] \;=\; \Omega m_{ij}^{+} .$$
(5.9)

These results imply that for $\widehat{\Lambda}$ itself to correspond to a physical density matrix, $\mathbf{n}$ must be a Hermitian matrix, since $\left\langle \widehat{b}_i^{\dagger}\widehat{b}_j \right\rangle^{*} = \left\langle \widehat{b}_j^{\dagger}\widehat{b}_i \right\rangle$, and $\mathbf{m}^{+}$ must be the Hermitian conjugate matrix of $\mathbf{m}$, since $\left\langle \widehat{b}_i\widehat{b}_j \right\rangle^{*} = \left\langle \widehat{b}_j^{\dagger}\widehat{b}_i^{\dagger} \right\rangle$. Physically, $\mathbf{n}$ gives the number, or normal, correlations, and $\mathbf{m}$ and $\mathbf{m}^{+}$ give the squeezing, or anomalous, correlations.

Another restriction on $\widehat{\Lambda}$ being a physical density matrix that follows from Eq. (5.9) is that the eigenvalues of the matrix $\mathbf{n}$ lie in the interval $[0, 1]$, because of the Pauli exclusion principle for fermions. Furthermore, the variance in the number correlations is

$$\mathrm{var}\left\{\left\langle \widehat{b}_i^{\dagger}\widehat{b}_j \right\rangle\right\} \;=\; \left\langle \widehat{b}_i^{\dagger}\widehat{b}_j \right\rangle\left(1 - \left\langle \widehat{b}_i^{\dagger}\widehat{b}_j \right\rangle\right), \quad (5.10)$$

which implies that if all the eigenvalues of $\mathbf{n}$ are 0 or 1, then $\widehat{\Lambda}$ is a number state, as the variance in number vanishes. If the eigenvalues are not limited to 0 or 1, then the $\widehat{\Lambda}$ corresponds to a mixture of number states in the eigenbasis and is thus a (possibly squeezed) thermal state, characterised by average occupation numbers $\overline{n}_j = \mathrm{eig}_j(\mathbf{n})$, and squeezing matrix $\mathbf{m}$.

A general Gaussian operator will not necessarily fulfill the Hermiticity condition and thus will not necessarily correspond to a physical state. However the set of operators that do correspond to physical states is an important subclass, because the expansion allows these states to be represented with exact precision. The inclusion of nonphysical operators in the expansion, on the other hand, makes the Gaussian basis an (over)complete basis in which to expand a physical density operator of an arbitrary state (This is proved below for the general case). The overcompleteness of the Gaussian operators as a basis set has important implications for representing arbitrary states with a positive distribution function, a fact that we discuss in detail elsewhere[15].

C. Completeness and Positivity

We next wish to show that the previous results on completeness and positivity obtained for one and two mode density matrix representations can be generalized to the multi-mode case. That is, we will prove that:

- For any physical density matrix $\hat{\rho}$, a positive set of coefficients P_j exists such that

$$\hat{\rho} = \sum_j P_j \widehat{\Lambda}(\underline{\underline{\sigma}}^{(j)}) \ . \tag{5.11}$$

This central result does not rely on utilising the complex amplitudes Ω, which are part of the most general Gaussian operator. If these were used, then positivity of the coefficients would be trivial, since these additional amplitudes could be used to absorb any phase or sign factors arising in the expansion. Instead, we wish to prove a much stronger result, that a positive expansion exists without any additional amplitude factors. This result is analogous to a similar result known for the positive-P bosonic representation[7, 8].

From the number state basis of Eq (2.2), the full set of possible fermionic many-body number states is the set $\{|\vec{n}\rangle\}$ where $\vec{n}$ is varied over all 2^M possible permutations. This defines a complete basis of 2^{2M} number-state projectors for the set of all fermionic density operators. While not all the number-state projectors are Hermitian, it is no restriction to use this larger set of operators as a basis for the density matrices $\hat{\rho}$.

Next, we expand:

$$\begin{aligned} \hat{\rho} &= \sum_{\vec{n}} \sum_{\vec{m}} |\vec{n}\rangle \langle\vec{n}| \hat{\rho} |\vec{m}\rangle \langle\vec{m}| \\ &= \sum_{\vec{n}} \sum_{\vec{m}} \rho_{\vec{n}\vec{m}} |\vec{n}\rangle \langle\vec{m}| \\ &= \sum_{\vec{n}} \sum_{\vec{m}} \hat{\rho}_{\vec{n}\vec{m}} \end{aligned} \tag{5.12}$$

The positive definiteness of the density operator means in particular that diagonal density matrix elements are real

and positive: $\rho_{\vec{n}\vec{n}} > 0$. It is sufficient for completeness to prove that any elementary fermionic operator of form $\hat{\rho}_{\vec{n}\vec{m}} = \rho_{\vec{n}\vec{m}} |\vec{n}\rangle \langle\vec{m}|$ corresponds to a normalised Gaussian $\widehat{\Lambda}(\vec{\lambda})$, apart from a positive scaling factor. The demonstration proceeds by constructing limiting cases of Gaussians that correspond to each of the elementary components of the density matrix. As demonstrated in the one and two mode cases, such expansions are not unique, and generally one can obtain other more compact representations by combining diagonal and off-diagonal elements.

To prove the elementary result, we proceed in three steps:

1. Diagonal operators

First, the generic diagonal operator in the number basis is:

$$\begin{aligned} \hat{\rho}_{\vec{n}\vec{n}} &= \rho_{\vec{n}\vec{n}} |\vec{n}\rangle \langle\vec{n}| \\ &= \rho_{\vec{n}\vec{n}} \prod_i |n_i\rangle_i \langle n_i|_i \ , \end{aligned} \tag{5.13}$$

with a total occupation number

$$N = \sum_i n_i \ . \tag{5.14}$$

Each diagonal multi-mode projector $|\vec{n}\rangle \langle\vec{n}|$ is simply an outer-product of single-mode density matrices. From the single-mode example in Section III A, each single-mode density matrix corresponds to a Gaussian as in Eq(3.6). Thus, we see that a diagonal projector is exactly equal to a normalized Gaussian (we suppress the trivial arguments for simplicity):

$$\begin{aligned} |\vec{n}\rangle \langle\vec{n}| &= \prod_i \widehat{\Lambda}_1 [n_i] \\ &= \widehat{\Lambda}_M [\mathbf{n}] \ , \end{aligned} \tag{5.15}$$

where the matrix $\mathbf{n}$ is defined as $n_{ij} = n_i \delta_{ij}$.

Because the $\rho_{\vec{n}\vec{n}}$ are real and positive, Eq. (5.13) shows that a positive Gaussian expansion exists for all diagonal density matrices:

$$\widehat{\rho}_{\vec{n}\vec{n}} = \rho_{\vec{n}\vec{n}} \widehat{\Lambda}_M [\mathbf{n}] \ . \tag{5.16}$$

In summary, a diagonal multi-mode projector $|\vec{n}\rangle \langle\vec{n}|$ is simply an outer-product of single-mode density matrices, and hence corresponds exactly to a multi-mode normalized Gaussian.

2. Generalized thermal operators

Next, consider off-diagonal projectors in the number-state expansion that conserve total number, i.e.

$$\widehat{\rho}_{\vec{n}\vec{m}} = \rho_{\vec{n}\vec{m}} |\vec{n}\rangle \langle\vec{m}| \ , \tag{5.17}$$

for which

$$\sum_i n_i = N = \sum_i m_i \ . \tag{5.18}$$

We show that any such component can be written as the limiting form of a number-conserving Gaussian, up to a positive scaling factor.

Let

$$n'_{ij} = \delta_{ij} \min\{n_i, m_i\}, \tag{5.19}$$

and define an off-diagonal Gaussian in terms of the diagonal normalized Gaussian:

$$\widehat{\Lambda}^{(o)}(\boldsymbol{\mu}, \mathbf{n}') = \ : \prod_{i \neq j} \left[1 - \mu_{ij} \hat{b}_i^\dagger \hat{b}_j\right] \widehat{\Lambda}\left[\mathbf{n}'\right] : \ . \tag{5.20}$$

Now for every distinct mode i with $\delta n_i = n_i - n'_i = 1$ one can define a corresponding distinct index $j(i)$ with $\delta m_j = m_j - m'_j = 1$. It follows from the minimum condition, Eq(5.19) that $j(i) \neq i$, and from the number-conservation equation, Eq (5.18), we have

$$\sum_i \delta n_i = \sum_i \delta m_i \ . \tag{5.21}$$

Similarly, for every distinct pairs of indices i, i' with $\delta n_i = \delta n_{i'} = 1$, it follows that $j(i') \neq i$, since otherwise $\delta n_i = 0$. The mapping therefore generates distinct pairs so that $j(i) \neq j(i') \iff i \neq i'$. Next, we note that this mapping is not a permutation of the set of modes i with $\delta n_i = 0$, since if it were the condition that $j(i') \neq i$ would be violated for some i'. Similarly, the mapping is not a permutation of any subset of these modes. This means that the only non-vanishing terms in the normalization factor $\det[2\mathbf{I} - \boldsymbol{\mu}]$ are the diagonal terms, which are already normalized.

Proceed by defining the resulting set of $\delta M \leq M$ pairs as $\sigma = \{i, j\}$, and let:

$$\mu_{ij}(\varepsilon, \vec{n}) = \sum_{\{i', j'\} \in \sigma} \frac{\mu \delta_{ii'} \delta_{jj'}}{-\varepsilon}$$

where $\mu^{\delta M} = \rho_{\vec{n}\vec{m}}$, so that:

$$\begin{aligned}
\widehat{\Lambda}[\boldsymbol{\mu}(\varepsilon), \mathbf{n}'] &= \ : \prod_{i \neq j} \left[1 - \mu_{ij} \hat{b}_i^\dagger \hat{b}_j\right] \widehat{\Lambda}\left[\mathbf{n}'\right] : \\
&= \ : \prod_{\{i,j\} \in \sigma} \left[1 + \frac{\mu \hat{b}_i^\dagger \hat{b}_j}{\varepsilon}\right] |\vec{n}'\rangle \langle \vec{n}'| :
\end{aligned} \tag{5.22}$$

Then consider the limit of $\varepsilon \to 0$, so that to leading order,

$$\begin{aligned}
\widehat{\rho}_{\vec{n}\vec{m}} &= \mu^{\delta M} \ : \prod_{\{i,j\} \in \sigma} \left[\hat{b}_i^\dagger \hat{b}_j\right] |\vec{n}'\rangle \langle \vec{n}'| : \\
&= \lim_{\varepsilon \to 0} \varepsilon^{\delta M} \widehat{\Lambda}[\boldsymbol{\mu}(\varepsilon), \mathbf{n}'] \tag{5.23}
\end{aligned}$$

Again, we see that a positive expansion parameter is obtained.

Finally, we consider the remaining elements of the density operator expansion, i.e. those squeezed projectors $\widehat{\rho}_{\vec{n}\vec{m}}$ for which

$$N = \sum_i n_i = \sum_i m_i + 2S \ , \tag{5.24}$$

where S is an integer denoting the change in the number of fermion pairs. We suppose that $S > 0$, since the case of $S < 0$ is obtained trivially by hermitian conjugation. Let $\widetilde{n}_i$ be obtained from n_i by removing $2S$ occupied sites, labeled as successive pairs i, j belonging to a set $\widetilde{\sigma}$, so that $\widetilde{N} = \sum_i \widetilde{n}_i = \sum_i m_i$. The occupation numbers $\widetilde{n}_i, m_i$ now define a generalised thermal density matrix component as previously, and hence equate to a limiting case of a Gaussian operator from Eq (5.23) above.

Now define a squeezed off-diagonal Gaussian in terms of the thermal case, which we have already proved has a positive representation:

$$\widehat{\Lambda}^{(s)}(\boldsymbol{\mu}(\varepsilon), \boldsymbol{\xi}(\varepsilon), \mathbf{n}') = \prod_{i > j} \left[1 - \xi_{ij} \hat{b}_i^\dagger \hat{b}_j^\dagger\right] \widehat{\Lambda}\left[\boldsymbol{\mu}(\varepsilon), \mathbf{n}'\right] \ , \tag{5.25}$$

where:

$$\xi_{ij}(\varepsilon) = \sum_{\{i', j'\} \in \widetilde{\sigma}} \frac{\delta_{ii'} \delta_{jj'}}{-\varepsilon} \ . \tag{5.26}$$

Then consider the limit of $\varepsilon \to 0$ as before, so that to leading order,

$$\begin{aligned}
\widehat{\rho}_{\vec{n}\vec{m}} &= \ : \prod_{\{i,j\} \in \widetilde{\sigma}} \left[\hat{a}_i^\dagger \hat{a}_j^\dagger\right] |\vec{n}'\rangle \langle \vec{m}| : \\
&= \lim_{\varepsilon \to 0} \varepsilon^{S + \delta M} \widehat{\Lambda}^{(s)}[\boldsymbol{\mu}(\varepsilon), \boldsymbol{\xi}(\varepsilon), \mathbf{n}'] \tag{5.27}
\end{aligned}$$

A positive expansion parameter is obtained here as well, thus completing the proof.

D. Differential Properties

In order to use the Gaussian basis in a time-evolution problem, we need to be able to map the evolution of the density operator onto an evolution of the expansion coefficients P_j. To achieve this, one must be able to write the action of ladder operators on a Gaussian basis element in differential form.

We can differentiate the Gaussian operators with respect to their parameters to get

$$\begin{aligned}
\frac{d}{d\Omega} \widehat{\Lambda} &= \ \frac{1}{\Omega} \widehat{\Lambda}, \\
\frac{d}{d\underline{\underline{\sigma}}} \widehat{\Lambda} &= \ \underline{\underline{\sigma}}^{-1} \widehat{\Lambda} - \underline{\underline{\sigma}}^{-1} : \widehat{\underline{\hat{b}}} \widehat{\underline{\hat{b}}}^\dagger \widehat{\Lambda} : \underline{\underline{\sigma}}^{-1}, \tag{5.28}
\end{aligned}$$

where the matrix derivative is defined as

$$\left(\frac{\partial}{\partial \underline{\underline{\sigma}}} \right)_{\mu, \nu} = \frac{\partial}{\partial \sigma_{\nu\mu}} , \qquad (5.29)$$

i. e. involving a transpose. These expressions for the derivative can be inverted to obtain the important identities:

$$\widehat{\Lambda} = \Omega \frac{\partial}{\partial \Omega} \widehat{\Lambda} ,$$

$$: \underline{\widehat{b}} \, \underline{\widehat{b}}^\dagger \widehat{\Lambda} : = \underline{\underline{\sigma}} \widehat{\Lambda} - \underline{\underline{\sigma}} \frac{\partial \widehat{\Lambda}}{\partial \underline{\underline{\sigma}}} \underline{\underline{\sigma}} , \qquad (5.30)$$

and thus we can write the normally ordered action of any pair of operators on a Gaussian as a first-order derivative. As theorems 5 and 6 in Appendix B show, there are analogous identities for antinormally ordered and mixed pairs:

$$\left\{ \underline{\widehat{b}} : \underline{\widehat{b}}^\dagger \widehat{\Lambda} : \right\} = -\underline{\underline{\sigma}} \widehat{\Lambda} + \left(\underline{\underline{\sigma}} - \underline{\underline{I}} \right) \frac{\partial \widehat{\Lambda}}{\partial \underline{\underline{\sigma}}} \underline{\underline{\sigma}} ,$$

$$\left\{ \underline{\widehat{b}} \, \underline{\widehat{b}}^\dagger \widehat{\Lambda} \right\} = \left(\underline{\underline{\sigma}} - \underline{\underline{I}} \right) \widehat{\Lambda} - \left(\underline{\underline{\sigma}} - \underline{\underline{I}} \right) \frac{\partial \widehat{\Lambda}}{\partial \underline{\underline{\sigma}}} \left(\underline{\underline{\sigma}} - \underline{\underline{I}} \right) . \qquad (5.31)$$

For the subset of Gaussian operators that correspond to (generalised) thermal states, i. e. $\mathbf{m}^+ = \mathbf{m} = \mathbf{0}$, we obtain a simpler set of differential identities:

$$\widehat{\boldsymbol{b}}^{\dagger T} \widehat{\boldsymbol{b}}^T \widehat{\Lambda} = \boldsymbol{n} \widehat{\Lambda} + (\boldsymbol{I} - \boldsymbol{n}) \frac{\partial \widehat{\Lambda}}{\partial \boldsymbol{n}} \boldsymbol{n} ,$$

$$\widehat{\Lambda} \widehat{\boldsymbol{b}}^{\dagger T} \widehat{\boldsymbol{b}}^T = \boldsymbol{n} \widehat{\Lambda} + \boldsymbol{n} \frac{\partial \widehat{\Lambda}}{\partial \boldsymbol{n}} (\boldsymbol{I} - \boldsymbol{n}) ,$$

$$\widehat{\boldsymbol{b}}^{\dagger T} \widehat{\Lambda} \widehat{\boldsymbol{b}}^T = (\boldsymbol{I} - \boldsymbol{n}) \widehat{\Lambda} + (\boldsymbol{I} - \boldsymbol{n}) \frac{\partial \widehat{\Lambda}}{\partial \boldsymbol{n}} (\boldsymbol{I} - \boldsymbol{n}) ,$$

$$\left(\widehat{\boldsymbol{b}} \widehat{\Lambda} \widehat{\boldsymbol{b}}^\dagger \right)^T = \boldsymbol{n} \widehat{\Lambda} - \boldsymbol{n} \frac{\partial \widehat{\Lambda}}{\partial \boldsymbol{n}} \boldsymbol{n} . \qquad (5.32)$$

The action of four ladder operators on a Gaussian operator can be obtained by applying the previous identities twice. Thus in a Gaussian expansion, any two-body interaction term can be written as a second-order differential operator. As we show in detail elsewhere[15], this central result allows the evolving density operator to be mapped to a Fokker-Planck equation for the expansion coefficients, thus enabling a Monte-Carlo sampling of the many-body quantum state.

VI. CONCLUSION

In summary, we have introduced here a generalised Gaussian operator basis, as a means of defining a phase-space representation for correlated fermionic states. As

special cases, the set of Gaussian operators include the density operators for thermal states and squeezed states, and thus the physics of the noninteracting Fermi gas and the BCS state is incorporated into the basis itself. Furthermore, the basis also includes more general operators, which ensure an overcompleteness that makes it possible to express any physical density operator as a probabilistic distribution over the Gaussian operators, without the need to use Grassmann algebra.

We have calculated the normalisation and moments, and proved completeness and positivity for the most general basis, and also for specific subsets, such as the number-conserving thermal basis. These results mean that the phase-space representation defined by the Gaussian operators can be used for first-principles simulations of many-body fermionic systems. The mapping from the quantum operator to the probabilistic c-number description is enabled by the Gaussian differential identities that have been derived here. The application of these identities will be dealt with elsewhere, when we consider the phase-space representation in more detail.

Appendix A: GRASSMANN ALGEBRA

This appendix introduces the basic concepts of non-commuting algebra and lists some results pertaining to Grassmann calculus and Fermi coherent states. These results are used in Appendix B to establish important properties of the Gaussian operators. Proofs and further discussion of these results can be found in the literature[16, 17, 18].

Let $\boldsymbol{\alpha}$ be a vector of M anticommuting (Grassmann) numbers, i.e.

$$[\alpha_i, \alpha_j]_+ = 0 . \qquad (A1)$$

Since $\alpha_j^2 = 0$, any function of Grassmann numbers can be at most linear in any one of its arguments. Thus, for example, the single mode exponential is

$$\exp(\alpha_j) = 1 + \alpha_j , \qquad (A2)$$

and a multimode exponential, e. g. $\exp\left(\sum \alpha_j\right)$ will be an ordered product of such single-mode exponentials.

The Grassmann numbers anticommute with all Fermi annihilation and creation operators, but commute with c-numbers and bosonic operators.

1. Grassmann Calculus

Differentiation of a single Grassmann variable is defined as

$$\frac{\partial}{\partial \alpha_i} \alpha_j = \delta_{ij} , \qquad (A3)$$

with the derivative of products obtained by the Grassmann chain rule:

$$\frac{\partial}{\partial \alpha_j} [f(\boldsymbol{\alpha})g(\boldsymbol{\alpha})] = \begin{cases} \frac{\partial f}{\partial \alpha_j} g + f \frac{\partial g}{\partial \alpha_j} & , \ f \text{ even} \\ \frac{\partial f}{\partial \alpha_j} g - f \frac{\partial g}{\partial \alpha_j} & , \ f \text{ odd} \end{cases} , (A4)$$

i. e. the derivative operator also anticommutes.

Grassmann integration is defined to be the same as differentiation, but written in a different way:

$$\int d\alpha_j = 0$$
$$\int \alpha_j \, d\alpha_j = 1 . \qquad (A5)$$

Multivariate integrals are ordered sequences of single-variable integrations, which can be written without ambiguity if the integration measure (as for a derivative) is also taken to be an anticommuting number. For an integral over all variables in a vector, we define the integration measure to be ordered in increasing numerical order: $d\boldsymbol{\alpha} \equiv d\alpha_1 ... d\alpha_N$.

Note that integrating a total derivative gives zero:

$$\int d\alpha_j \frac{\partial}{\partial \alpha_j} f = 0 . \qquad (A6)$$

This fact, coupled with the product rule, gives a result for partial integration:

$$\int d\alpha_j \frac{\partial f}{\partial \alpha_j} g = \begin{cases} -\int d\alpha_j f \frac{\partial g}{\partial \alpha_j} & , \ f \text{ even} \\ \int d\alpha_j f \frac{\partial g}{\partial \alpha_j} & , \ f \text{ odd} \end{cases} . \quad (A7)$$

One very useful result is the multivariate Gaussian integral:

$$\int \exp\left(-\boldsymbol{\alpha}^T \mathbf{A} \boldsymbol{\alpha}/2\right) d\boldsymbol{\alpha} = \mathrm{Pf}\,[\mathbf{A}] \qquad (A8)$$

for an antisymmetric matrix $\mathbf{A}$ of complex numbers. The Pfaffian is related to the determinant $(\mathrm{Pf}\,[\mathbf{A}])^2 = \det \mathbf{A}$, and thus, apart from a sign change, has many of the same properties. For example, $\mathrm{Pf}\,[\mathbf{A}^T] = (-1)^N \mathrm{Pf}\,[\mathbf{A}]$ and $|\mathrm{Pf}\,[\mathbf{A}^{-1}]| = |1/\mathrm{Pf}\,[\mathbf{A}]|$. Another useful type of Gaussian integral is:

$$\int \exp\left(-\boldsymbol{\beta}^T \mathbf{B} \boldsymbol{\alpha}\right) \prod_{j=1}^{M} (d\beta_j d\alpha_j) = \det[\mathbf{B}] , \quad (A9)$$

where $\mathbf{B}$ is a square matrix of complex numbers and $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ are two independent Grassmann vectors. This second integral is in fact a special case of the first, except with $2M$ total Grassmann variables.

2. Grassmann coherent states

For each Grassmann number α_j we can associate another Grassmann number, denoted $\overline{\alpha}_j$, to play the role of a complex conjugate. This is formally regarded as an independent variable for calculus purposes. The conjugates $\overline{\alpha}_j$ anticommute with all other Grassmann variables. By use of such a complex Grassmann algebra, we can define a fermionic coherent state, which is formally an eigenstate of the annihilation operator:

$$|\alpha_j\rangle = (1 + \overline{\alpha}_j \alpha_j)^{-\frac{1}{2}} (|0\rangle + |1\rangle \alpha_j)$$
$$= \exp\left(\widehat{b}_j^\dagger \alpha_j - \frac{1}{2} \overline{\alpha}_j \alpha_j\right) |0\rangle , \qquad (A10)$$

$$\langle \alpha_j| = (1 + \overline{\alpha}_j \alpha_j)^{-\frac{1}{2}} (\langle 0| + \overline{\alpha}_j \langle 1|)$$
$$= \exp\left(\overline{\alpha}_j \widehat{b}_j - \frac{1}{2} \overline{\alpha}_j \alpha_j\right) \langle 0| . \qquad (A11)$$

Like the bosonic coherent state, the fermionic coherent state can be written as (Grassmann) displacement from the vacuum:

$$|\alpha_j\rangle = \exp\left(\widehat{b}_j^\dagger \alpha_j - \overline{\alpha}_j \widehat{b}_j\right) |0\rangle . \qquad (A12)$$

Multimode coherent states are products of the single-mode states:

$$|\boldsymbol{\alpha}\rangle = \prod_{j=1}^{M} |\alpha_j\rangle$$
$$= \exp\left[\left(\sum_{j=1}^{M} \widehat{b}_j^\dagger \alpha_j - \overline{\alpha}_j \widehat{b}_j\right)\right] |0\rangle$$

The inner product of two states is:

$$\langle \alpha_i | \alpha_j \rangle = \exp\left(\overline{\alpha}_i \alpha_j - \overline{\alpha}_i \alpha_i/2 - \overline{\alpha}_j \alpha_j/2\right) , (A13)$$

and thus as two special cases:

$$\langle \alpha_i | \alpha_i \rangle = 1$$
$$\langle -\alpha_i | \alpha_i \rangle = \exp\left(-2\overline{\alpha}_i \alpha_i\right) . \qquad (A14)$$

The usefulness of the coherent states lies in the fact that they form a complete set:

$$\int d\overline{\alpha}_j d\alpha_j \, |\alpha_j\rangle\langle \alpha_j| = |0\rangle\langle 0| + |1\rangle_j\langle 1| = I_1 , (A15)$$

or, for the multimode case,

$$\int d\underline{\alpha} \, |\boldsymbol{\alpha}\rangle\langle \boldsymbol{\alpha}| = I_M , \qquad (A16)$$

where we have defined a $2M$-variate integration measure as

$$d\underline{\alpha} \equiv \prod_{j=1}^{M} (d\overline{\alpha}_j d\alpha_j) . \qquad (A17)$$

Finally, we can express the trace of an arbitrary operator $\widehat{O}$ as

$$\text{Tr}\left[\widehat{O}\right] \;=\; \int d\underline{\alpha}\,\langle-\boldsymbol{\alpha}|\,\widehat{O}\,|\boldsymbol{\alpha}\rangle \;. \tag{A18}$$

Appendix B: GAUSSIAN FERMION OPERATORS

We prove some useful results concerning the most general multi-mode Gaussian operator constructed from fermionic ladder operators. The proofs make use of the properties of Grassmann coherent states and anticommuting algebra, which are summarized in Appendix A. However the final results do not contain any Grassmann variables. The results establish the trace and differential properties of the Gaussian operators that are discussed in Sec. V.

1. General Gaussian Operator

In this appendix, we use the vector and ordering notations introduced in Sec. IV. We find it convenient to use an unnormalised Gaussian form of Fermi operators:

$$\begin{aligned}
\widehat{\Lambda}^{(u)}(\underline{\underline{\mu}}) \;&=\; :\exp\left[-\widehat{\underline{b}}^{\dagger}\,\underline{\underline{\mu}}\,\widehat{\underline{b}}/2\right]:, \\
&\equiv\; \sum_{n=0}^{\infty}\frac{1}{2^{n}n!}:\left(-\widehat{\underline{b}}^{\dagger}\,\underline{\underline{\mu}}\,\widehat{\underline{b}}\right)^{n}: \\
&=\; :\prod_{\mu,\nu=1}^{2M}\left(1-\frac{1}{2}\widehat{b}_{\mu}^{\dagger}\,\mu_{\mu\nu}\,\widehat{b}_{\nu}\right): , \tag{B1}
\end{aligned}$$

where $\underline{\underline{\mu}}$ is a $2M\times 2M$ matrix of parameters, given by

$$\underline{\underline{\mu}} \;=\; \begin{bmatrix} \boldsymbol{\mu} & \boldsymbol{\xi} \\ \boldsymbol{\xi}^{+} & -\boldsymbol{\mu}^{T} \end{bmatrix}.$$

In terms of the covariance matrix $\underline{\underline{\sigma}}$, the unnormalised Gaussian is:

$$\widehat{\Lambda}^{(u)}(\underline{\underline{\sigma}}) \;=\; :\exp\left[\widehat{\underline{b}}^{\dagger}\left(\underline{\underline{I}}-\underline{\underline{\sigma}}^{-1}/2\right)\widehat{\underline{b}}\right]: , \tag{B2}$$

where the relation between the two parametrizations is $\underline{\underline{\sigma}}=[\underline{\underline{\mu}}+2\underline{\underline{I}}]^{-1}$ and where the diagonal matrix $\underline{\underline{I}}$ is as defined in Eq. (4.5).

Because of the anticommuting property of fermions, both $\underline{\underline{\sigma}}$ and $\underline{\underline{\mu}}$ possess a generalized antisymmetry: $\underline{\underline{\sigma}}=-\underline{\underline{\sigma}}^{+}$, $\underline{\underline{\mu}}=-\underline{\underline{\mu}}^{+}$, or more in block matrix form,

$$\begin{aligned}
\begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{bmatrix} \;&\equiv\; -\underline{\underline{X}}\begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{bmatrix}^{T}\underline{\underline{X}} \\
&=\; -\begin{bmatrix} \mathbf{d}^{T} & \mathbf{b}^{T} \\ \mathbf{c}^{T} & \mathbf{a}^{T} \end{bmatrix}, \tag{B3}
\end{aligned}$$

where the constant matrix $\underline{\underline{X}}$ is defined as

$$\underline{\underline{X}} \;\equiv\; \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix}. \tag{B4}$$

When applied to the left of a matrix, $\underline{\underline{X}}$ swaps the upper and lower halves; when applied to the right, it swaps the left and right halves. This structure means that the matrices $\underline{\underline{\sigma}}$ and $\underline{\underline{\mu}}$ can be transformed into explicitly antisymmetric forms by certain permutations of rows and columns. For example, it follows immediately from Eq. (B3) that interchanging left and right halves, or upper and lower halves, will generate an antisymmetric matrix. Alternatively, inserting each row in the lower half after the corresponding row in the upper half, and inserting each column in the right half before the corresponding row in the left half generates the antisymmetric form

$$\begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{bmatrix}_{A} \;\equiv\; \begin{bmatrix} b_{11} & a_{11} & \cdots & b_{1M} & a_{1M} \\ d_{11} & c_{11} & \cdots & d_{1M} & c_{1M} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ b_{M1} & a_{M1} & \cdots & b_{MM} & a_{MM} \\ d_{M1} & c_{M1} & \cdots & d_{MM} & c_{MM} \end{bmatrix}. \tag{B5}$$

With the covariance matrix antisymmetrized in this way, the Gaussian operator becomes

$$\widehat{\Lambda}^{(u)}(\underline{\underline{\sigma}}_{A}) \;=\; :\exp\left[\widehat{\underline{b}}_{A}^{T}\left(\underline{\underline{I}}_{A}-\underline{\underline{\sigma}}_{A}^{-1}/2\right)\widehat{\underline{b}}_{A}\right]: , \tag{B6}$$

where the vector of operators is now

$$\widehat{\underline{b}}_{A} \;=\; \begin{pmatrix} \widehat{b}_{1} \\ \widehat{b}_{1}^{\dagger} \\ \vdots \\ \widehat{b}_{M} \\ \widehat{b}_{M}^{\dagger} \end{pmatrix}. \tag{B7}$$

The generalised antisymmetry of $\underline{\underline{\sigma}}$ and $\underline{\underline{\mu}}$ has implications for matrix derivatives. Because each element of the matrix appears twice, we have $\partial\sigma_{\mu\nu}/\partial\sigma_{\theta\phi}=\delta_{\mu\theta}\delta_{\nu\phi}-X_{\mu\phi}X_{\nu\theta}$, where $\delta_{\mu\nu}$ is the Kronecker delta function. The extra terms here appear in the derivative of an inverse:

$$\frac{\partial\sigma_{\mu\nu}^{-1}}{\partial\sigma_{\theta\phi}} \;=\; -\sigma_{\mu\theta}^{-1}\sigma_{\phi\nu}^{-1}+\sigma_{\mu\gamma}^{-1}X_{\gamma\phi}X_{\theta\epsilon}\sigma_{\epsilon\nu}^{-1}, \tag{B8}$$

and they also give an additional factor of two in the derivative of a determinant, thus:

$$\frac{d}{d\underline{\underline{\sigma}}}\sqrt{\det\underline{\underline{\sigma}}} \;=\; \sqrt{\det\underline{\underline{\sigma}}}\,\underline{\underline{\sigma}}^{-1}, \tag{B9}$$

where we define the matrix derivative as

$$\left(\frac{d}{d\underline{\underline{\sigma}}}\right)_{\mu\nu} \;=\; \frac{d}{d\sigma_{\nu\mu}}, \tag{B10}$$

i. e. involving a transpose. The result (B8) allows us to relate the derivatives with respect to $\underline{\sigma}$ and $\underline{\mu}$:

$$\frac{df}{d\underline{\mu}} = \frac{df}{d\underline{\sigma}^{-1}} = -\underline{\sigma}\frac{df}{d\underline{\sigma}}\underline{\sigma}. \quad \text{(B11)}$$

2. Normalisation

Theorem 1: The trace of the unnormalised Gaussian operator is equal to the Pfaffian of the inverse of the antisymmetrized covariance, i. e.

$$N \equiv \text{Tr}\left[\widehat{\Lambda}^{(u)}(\underline{\sigma})\right] = \text{Pf}\left[\underline{\underline{\sigma}}_A^{-1}\right], \quad \text{(B12)}$$

where Pf stands for Pfaffian.

Proof: Because the Gaussian is in normally ordered form, it is straightforward to evaluate the trace with multimode Grassmann coherent states $|\boldsymbol{\alpha}\rangle$, using the Grassmann trace result of Eq. (A18):

$$\text{Tr}\left[\widehat{\Lambda}^{(u)}\right] = \int \langle-\boldsymbol{\alpha}|\widehat{\Lambda}^{(u)}|\boldsymbol{\alpha}\rangle \prod_j^M [d\overline{\alpha}_j d\alpha_j]$$
$$= \int \exp\left[-\underline{\alpha}^\dagger\underline{\sigma}^{-1}\underline{\alpha}/2\right] \prod_j^M [-d\overline{\alpha}_j d\alpha_j], \quad \text{(B13)}$$

where we have made use of the fact that, from the Grassmann inner product result of Eq. (A13), $\langle-\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle = \exp(-2\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha})$. We have also changed variables: $\overline{\alpha}_j \rightarrow -\overline{\alpha}_j$, and introduced $2M$-vectors of Grassmann variables $\underline{\alpha} = (\boldsymbol{\alpha}, (\overline{\boldsymbol{\alpha}})^T)$ and $\underline{\alpha}^\dagger = (\overline{\boldsymbol{\alpha}}, \boldsymbol{\alpha}^T)$. Changing to the antisymmetric form of the covariance $\underline{\underline{\sigma}}_A$, and swapping the order of the pairs in the integration measure, we obtain

$$\text{Tr}\left[\widehat{\Lambda}^{(u)}\right] = \int \exp\left[-\underline{\alpha}_A^T\underline{\underline{\sigma}}_A^{-1}\underline{\alpha}_A/2\right] \prod_j^M [d\alpha_j d\overline{\alpha}_j], \quad \text{(B14)}$$

where the reordered Grassmann vector is $\underline{\alpha}_A = (\alpha_1, \overline{\alpha}_1, ..., \alpha_M, \overline{\alpha}_M)^T$. Noting that the arrangement of elements in $\underline{\alpha}_A$ matches the order of integration, we can apply the Gaussian integral result [Eq. A8]:

$$\text{Tr}\left[\widehat{\Lambda}^{(u)}\right] = \text{Pf}\left[\underline{\underline{\sigma}}_A^{-1}\right]. \quad \text{(B15)}$$

QED.

Corollaries:
Now the square of the Pfaffian of a matrix is equal to its determinant. Thus, to within a $\pm$ sign, the normalisation

is determined by the determinant of the covariance:

$$\left(\text{Tr}\left[\widehat{\Lambda}^{(u)}\right]\right)^2 = \frac{1}{\det\left[\underline{\underline{\sigma}}_A\right]} = \frac{(-1)^M}{\det\left[\underline{\sigma}\right]} = \frac{1}{\det\left[i\underline{\sigma}\right]}, \quad \text{(B16)}$$

and thus we may write the Gaussian operator in normalised form as

$$\widehat{\Lambda} = \pm\sqrt{\det\left[i\underline{\sigma}\right]} : \exp\left[\widehat{\underline{b}}^\dagger\left(\underline{I} - \underline{\sigma}^{-1}/2\right)\widehat{\underline{b}}\right] :, \quad \text{(B17)}$$

where the choice of plus/minus sign is determined by $\sqrt{\det\left[\underline{\underline{\sigma}}_A\right]}\text{Pf}\left[\underline{\underline{\sigma}}_A^{-1}\right]$. This extra sign, or phase, which does not appear in the normalizations of the familiar complex-number or bosonic Gaussians, fortunately does not appear in any of the identities needed to make use of the Gaussian operators as a basis for a phase-space representation.

A specific case where the determinant appears is for the generalised thermal Gaussian without squeezing parameters, so that $\mathbf{m} = \mathbf{m}^+ = 0$. In this case, the normalization follows directly from the second Grassmann Gaussian integral identity, Eq. (A9). Following the same procedure as before, we find that:

$$\text{Tr}\left[\widehat{\Lambda}^{(u)}\right] = \det\left[2\boldsymbol{I} - \boldsymbol{\mu}\right]. \quad \text{(B18)}$$

3. First-order moments

Theorem 2: The fermionic Gaussian operator is completely characterised by its first-order moments. In particular, the covariance matrix corresponds to the first-order moments in normally ordered trace form, i. e.

$$\text{Tr}\left[:\widehat{\underline{b}}\widehat{\underline{b}}^\dagger\widehat{\Lambda}:\right] = \underline{\sigma}, \quad \text{(B19)}$$

where $\widehat{\underline{b}}\widehat{\underline{b}}^\dagger$ is a matrix multiplication of two vectors, resulting in the $2M \times 2M$ matrix of Eq. (4.2).
Proof: We proceed as in the proof of Theorem 1, by taking the trace of the unnormalised form using Grassmann coherent states and then changing variables: $\overline{\alpha}_j \rightarrow -\overline{\alpha}_j$:

$$\text{Tr}\left[:\widehat{\underline{b}}\widehat{\underline{b}}^\dagger\widehat{\Lambda}^{(u)}:\right] = \int \langle-\boldsymbol{\alpha}|:\widehat{\underline{b}}\widehat{\underline{b}}^\dagger\widehat{\Lambda}^{(u)}:|\boldsymbol{\alpha}\rangle \prod_j^M [d\overline{\alpha}_j d\alpha_j]$$
$$= \int \underline{\alpha}\,\underline{\alpha}^\dagger \exp\left[-\underline{\alpha}^\dagger\underline{\sigma}^{-1}\underline{\alpha}/2\right] \prod_j^M [d\alpha_j d\overline{\alpha}_j]. \quad \text{(B20)}$$

Next we put the integral into the form Eq. (A8):

$$\text{Tr}\left[: \widehat{\underline{b}}\,\widehat{\underline{b}}^\dagger\,\widehat{\Lambda}^{(u)}:\right]=$$

$$\int -\left(\underline{\alpha}^{\dagger T}\,\underline{\alpha}^T\right)^T \exp\left[-\underline{\alpha}^\dagger\,\underline{\underline{\sigma}}^{-1}\,\underline{\alpha}/2\right]\prod_j^M [d\alpha_j d\overline{\alpha}_j]$$

$$= \frac{d}{d\underline{\underline{\sigma}}^{-1}}\int \exp\left[-\underline{\alpha}^\dagger\,\underline{\underline{\sigma}}^{-1}\,\underline{\alpha}/2\right]\prod_j^M [d\alpha_j d\overline{\alpha}_j]\ ,\quad \text{(B21)}$$

where in taking the derivative with respect to $\underline{\underline{\sigma}}^{-1}$ we have taken account of the fact that each element of it appears twice, owing to its generalized antisymmetry. Evaluating the Grassmann integral, and employing the determinant result , we get

$$\text{Tr}\left[: \widehat{\underline{b}}\,\widehat{\underline{b}}^\dagger\,\widehat{\Lambda}^{(u)}:\right] = \frac{d}{d\underline{\underline{\sigma}}^{-1}}(\pm)\sqrt{\det\left[i\underline{\underline{\sigma}}^{-1}\right]}$$

$$= \pm\sqrt{\det\left[i\underline{\underline{\sigma}}^{-1}\right]}\underline{\underline{\sigma}}\ .\quad \text{(B22)}$$

Finally, dividing through by the normalisation in Eq. (B12) gives the normalised result . QED.

Corollaries:

We can put Eq. (B19) into a more familiar form by using the cyclic property of trace:

$$\text{Tr}\left[: \widehat{\underline{b}}\,\widehat{\underline{b}}^\dagger\,\widehat{\Lambda}:\right] = \text{Tr}\left[\begin{array}{cc} -\left(\widehat{\mathbf{b}}^{\dagger T}\widehat{\Lambda}\widehat{\mathbf{b}}^T\right)^T & \widehat{\Lambda}\widehat{\mathbf{b}}\widehat{\mathbf{b}}^T \\ \widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^\dagger\widehat{\Lambda} & \widehat{\mathbf{b}}^{\dagger T}\widehat{\Lambda}\widehat{\mathbf{b}}^T \end{array}\right]$$

$$= \text{Tr}\left[\begin{array}{cc} -\widehat{\mathbf{b}}\widehat{\mathbf{b}}^\dagger & \widehat{\mathbf{b}}\widehat{\mathbf{b}}^T \\ \widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^\dagger & \left(\widehat{\mathbf{b}}\widehat{\mathbf{b}}^\dagger\right)^T \end{array}\right]\widehat{\Lambda}$$

$$= \left[\begin{array}{cc} \mathbf{n}^T - \mathbf{I} & \mathbf{m} \\ \mathbf{m}^+ & \mathbf{I} - \mathbf{n} \end{array}\right]\ ,\quad \text{(B23)}$$

where we have defined the matrix $\mathbf{n}$ for the number, or normal, moments, and the matrices $\mathbf{m}$ and $\mathbf{m}^+$ for the squeezing, or anomalous, moments, as follows:

$$\mathbf{n} = \left\langle \widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^T \right\rangle_{\widehat{\Lambda}}\ ,$$

$$\mathbf{m} = \left\langle \widehat{\mathbf{b}}\widehat{\mathbf{b}}^T \right\rangle_{\widehat{\Lambda}}\ ,$$

$$\mathbf{m}^+ = \left\langle \widehat{\mathbf{b}}^{\dagger T}\widehat{\mathbf{b}}^\dagger \right\rangle_{\widehat{\Lambda}}\ ,\quad \text{(B24)}$$

where $\left\langle \widehat{O} \right\rangle_{\widehat{\Lambda}} \equiv \text{Tr}\left[\widehat{O}\,\widehat{\Lambda}\right]$. Thus we can write covariance matrix in terms of the moments as

$$\underline{\underline{\sigma}} = \left[\begin{array}{cc} \mathbf{n}^T - \mathbf{I} & \mathbf{m} \\ \mathbf{m}^+ & \mathbf{I} - \mathbf{n} \end{array}\right]\ ,\quad \text{(B25)}$$

or inverting the relationship,

$$\left\langle : \widehat{\underline{b}}\,\widehat{\underline{b}}^\dagger : \right\rangle_{\widehat{\Lambda}} = \underline{I} - \underline{I}\,\underline{\underline{\sigma}}\,\underline{I}\ .\quad \text{(B26)}$$

4. Higher-order moments

One can calculate higher-order moments along similar lines, i. e. by expanding the trace as a Grassmann integral then converting this into a higher-order derivative of a determinant. The results of this procedure in the general case can be written in terms of a moment generating function.

Theorem 3: Any even moment of a Gaussian operator, in normally ordered trace form, can be calculated by means of the moment generating function

$$M(\underline{\underline{\tau}}) \equiv \sqrt{\det\left[\underline{I}^2 - \underline{\underline{\sigma}}\,\underline{\underline{\tau}}\right]}\quad \text{(B27)}$$

as follows

$$\text{Tr}\left[: \widehat{b}^\dagger_{\mu_1}\widehat{b}_{\mu_2}\cdots \widehat{b}^\dagger_{\mu_{r-1}}\widehat{b}_{\mu_r}\widehat{\Lambda}:\right] = \frac{\partial}{\partial\tau_{\mu_1,\mu_2}}\cdots$$

$$\cdots \frac{\partial}{\partial\tau_{\mu_{r-1},\mu_r}}M(\underline{\underline{\tau}})\Big|_{\underline{\underline{\tau}}=0}\ .\quad \text{(B28)}$$

Proof: We start by writing the normally ordered operator product as a derivative of a normally ordered Gaussian:

$$: \widehat{b}^\dagger_{\mu_1}\widehat{b}_{\mu_2}\cdots \widehat{b}^\dagger_{\mu_{r-1}}\widehat{b}_{\mu_r}: = \frac{\partial}{\partial\tau_{\mu_1,\mu_2}}\cdots\frac{\partial}{\partial\tau_{\mu_{r-1},\mu_r}}$$

$$: \exp\left[\widehat{\underline{b}}^+\,\underline{\underline{\tau}}\,\widehat{\underline{b}}/2\right]:\Big|_{\underline{\underline{\tau}}=0}\quad \text{(B29)}$$

where $\underline{\underline{\tau}}$ is a $2M \times 2M$ matrix of complex numbers with the generalised antisymmetry $\underline{\underline{\tau}} = -\underline{\underline{\tau}}^+$. Using this result in Eq. (B28) shows that the moment generating function $M(\underline{\underline{\tau}})$ must satisfy

$$M(\underline{\underline{\tau}}) = \text{Tr}\left[: \exp\left(\widehat{\underline{b}}^+\,\underline{\underline{\tau}}\,\widehat{\underline{b}}/2\right)\widehat{\Lambda}:\right],\quad \text{(B30)}$$

which can be evaluated by writing the trace as a Grassmann integral

$$M(\underline{\underline{\tau}}) = \frac{1}{N}\int \exp\left[-\underline{\alpha}^\dagger\left(\underline{\underline{\sigma}}^{-1} - \underline{\underline{\tau}}\right)\underline{\alpha}/2\right]\prod_j^M [d\alpha_j d\overline{\alpha}_j]\ .\quad \text{(B31)}$$

Using the Gaussian integral result (A8), we get

$$M(\underline{\underline{\tau}}) = \text{Pf}\left[\underline{\underline{\sigma}}_A^{-1} - \underline{\underline{\tau}}_A\right]/\text{Pf}\left[\underline{\underline{\sigma}}_A^{-1}\right]\ .\quad \text{(B32)}$$

Because of the relationship between Pfaffians and determinants, we can rewrite this as

$$M(\underline{\underline{\tau}}) = \sqrt{\det\left[\underline{\underline{\sigma}}_A^{-1} - \underline{\underline{\tau}}_A\right]}/\sqrt{\det\left[\underline{\underline{\sigma}}_A^{-1}\right]}$$

$$= \sqrt{\det\left[\underline{I}^2 - \underline{\underline{\sigma}}\,\underline{\underline{\tau}}\right]},\quad \text{(B33)}$$

where the sign of the square root is chosen to give a positive result when $\underline{\tau} = 0$. QED

Examples:

To calculate the derivatives of the moment generating function, one makes use of the results for the derivative of a determinant Eq. (B9) and of an inverse Eq. (B8). A general second-order moment is of the form

$$\text{Tr}\left[: \widehat{b}_{\mu_1}\widehat{b}_{\mu_2}^{\dagger}\widehat{b}_{\mu_3}\widehat{b}_{\mu_4}^{\dagger}\widehat{\Lambda} :\right] = \sigma_{\mu_1\mu_2}\sigma_{\mu_3\mu_4} - \sigma_{\mu_1\mu_4}\sigma_{\mu_3\mu_2} + (\sigma X)_{\mu_1\mu_3}(X\sigma)_{\mu_4\mu_2}. \quad (B34)$$

Thus the normally ordered number-number correlations are

$$\text{Tr}\left[: \widehat{n}_i\widehat{n}_j : \widehat{\Lambda}\right] = n_{ii}n_{jj} - n_{ij}n_{ji} - m_{ij}m_{ij}^{+}, \quad (B35)$$

i. e. containing the three terms expected for a state with Gaussian correlations.

Similarly, a third-order moment is of the form

$$\text{Tr}\left[: \widehat{b}_{\mu_1}\widehat{b}_{\mu_2}^{\dagger}\widehat{b}_{\mu_3}\widehat{b}_{\mu_4}^{\dagger}\widehat{b}_{\mu_5}\widehat{b}_{\mu_6}^{\dagger}\widehat{\Lambda} :\right] =$$

$$\sigma_{\mu_1\mu_2}\sigma_{\mu_3\mu_6}\sigma_{\mu_5\mu_4} + \sigma_{\mu_1\mu_4}\sigma_{\mu_3\mu_2}\sigma_{\mu_5\mu_6} + \sigma_{\mu_1\mu_6}\sigma_{\mu_3\mu_4}\sigma_{\mu_5\mu_2}$$
$$- \sigma_{\mu_1\mu_2}\sigma_{\mu_3\mu_4}\sigma_{\mu_5\mu_6} - \sigma_{\mu_1\mu_4}\sigma_{\mu_3\mu_6}\sigma_{\mu_5\mu_2} - \sigma_{\mu_1\mu_6}\sigma_{\mu_3\mu_2}\sigma_{\mu_5\mu_4}$$
$$- \sigma_{\mu_1\mu_2}(\sigma X)_{\mu_3\mu_5}(X\sigma)_{\mu_6\mu_4} - \sigma_{\mu_3\mu_4}(\sigma X)_{\mu_1\mu_5}(X\sigma)_{\mu_6\mu_2}$$
$$- \sigma_{\mu_5\mu_6}(\sigma X)_{\mu_1\mu_3}(X\sigma)_{\mu_4\mu_2} + \sigma_{\mu_1\mu_4}(\sigma X)_{\mu_3\mu_5}(X\sigma)_{\mu_6\mu_2}$$
$$- \sigma_{\mu_1\mu_6}(\sigma X)_{\mu_3\mu_5}(X\sigma)_{\mu_4\mu_2} + \sigma_{\mu_3\mu_2}(\sigma X)_{\mu_1\mu_5}(X\sigma)_{\mu_6\mu_4}$$
$$+ \sigma_{\mu_3\mu_6}(\sigma X)_{\mu_1\mu_5}(X\sigma)_{\mu_4\mu_2} - \sigma_{\mu_5\mu_2}(\sigma X)_{\mu_1\mu_3}(X\sigma)_{\mu_6\mu_4}$$
$$+ \sigma_{\mu_5\mu_4}(\sigma X)_{\mu_1\mu_3}(X\sigma)_{\mu_6\mu_2}. \quad (B36)$$

Thus the normally ordered triple correlations are:

$$\text{Tr}\left[: \widehat{n}_i\widehat{n}_j\widehat{n}_k : \widehat{\Lambda}\right] = n_{ii}n_{jj}n_{kk} - n_{ii}\left(n_{jk}n_{kj} + m_{jk}m_{jk}^{+}\right)$$
$$+ n_{ij}n_{jk}n_{ki} - n_{jj}\left(n_{ik}n_{ki} + m_{ik}m_{ik}^{+}\right)$$
$$+ n_{ji}n_{kj}n_{ik} - n_{kk}\left(n_{ij}n_{ji} + m_{ij}m_{ij}^{+}\right)$$
$$+ n_{ij}m_{ik}m_{jk}^{+} + n_{ji}m_{jk}m_{ik}^{+}$$
$$+ n_{jk}m_{ji}m_{ki}^{+} + n_{kj}m_{ki}m_{ji}^{+}$$
$$+ n_{ki}m_{kj}m_{ij}^{+} + n_{ik}m_{kj}m_{ij}^{+}, \quad (B37)$$

again as expected for a state with Gaussian correlations.

5. Normally ordered products

Theorem 4: A normally ordered product of a pair of ladder operators and a Gaussian is equivalent to a first-order differential operator on the Gaussian, as follows:

$$: \widehat{\underline{b}}\,\widehat{\underline{b}}^{\dagger}\widehat{\Lambda} : = \underline{\sigma}\widehat{\Lambda} - \underline{\sigma}\frac{\partial\widehat{\Lambda}}{\partial\underline{\sigma}}\underline{\sigma}. \quad (B38)$$

Proof: The proof can be established easily without Grassmann algebra. We first take the derivative of the unnormalised Gaussian operator:

$$\frac{\partial}{\partial\mu_{\mu\nu}}\widehat{\Lambda}^{(u)}(\underline{\mu}) = - : \widehat{b}_{\mu}^{\dagger}\widehat{\Lambda}^{(u)}(\underline{\mu})\widehat{b}_{\nu} : . \quad (B39)$$

We write this as a derivative with respect to the covariance matrix, using Eq. (B11), and swap the pair of operators, to give,

$$\underline{\sigma}\frac{d\widehat{\Lambda}^{(u)}(\underline{\sigma})}{d\underline{\sigma}}\underline{\sigma} = - : \widehat{\underline{b}}\,\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}^{(u)}(\underline{\sigma}) : . \quad (B40)$$

Next, we take the derivative of the normalisation, using Eq. (B9):

$$\frac{d}{d\underline{\sigma}}N = \frac{d}{d\underline{\sigma}}(\pm)\left(\det[i\underline{\sigma}]\right)^{-\frac{1}{2}}$$
$$= -N\underline{\sigma}^{-1}. \quad (B41)$$

Combining both of these results, we find that the derivative of the normalised Gaussian is

$$\frac{d}{d\underline{\sigma}}\widehat{\Lambda} = -N^{-2}\widehat{\Lambda}^{(u)}\frac{dN}{d\underline{\sigma}} + N^{-1}\frac{d}{d\underline{\sigma}}\widehat{\Lambda}^{(u)}$$
$$= \underline{\sigma}^{-1}\widehat{\Lambda} - \underline{\sigma}^{-1} : \widehat{\underline{b}}\,\widehat{\underline{b}}^{\dagger}\widehat{\Lambda} : \underline{\sigma}^{-1}, \quad (B42)$$

whose inverse is the required result. QED.

This result can also be proved by use of Grassmann coherent-state expansions, in similar manner to the proofs below for the products of different ordering.

6. Mixed products

Theorem 5: A product of mixed order of a pair of ladder operators and a Gaussian is equivalent to a first-order differential operator on the Gaussian, as follows:

$$\left\{\widehat{\underline{b}} : \widehat{\underline{b}}^{\dagger}\widehat{\Lambda} :\right\} = -\underline{\sigma}\widehat{\Lambda} + \left(\underline{\sigma} - \underline{I}\right)\frac{\partial\widehat{\Lambda}}{\partial\underline{\sigma}}\underline{\sigma}. \quad (B43)$$

Proof: We first make use of the Fermi coherent-state completeness identity to replace all ladder operators by Grassmann integrals over coherent projection operators:
$$\left\{\widehat{\underline{b}} : \widehat{\underline{b}}^{\dagger}\widehat{\Lambda} :\right\} =$$

$$\int d\underline{\gamma}d\underline{\beta}d\underline{\alpha}d\underline{\epsilon}\,|\boldsymbol{\gamma}\rangle\langle\boldsymbol{\gamma}|\left\{\widehat{\underline{b}} : |\boldsymbol{\beta}\rangle\langle\boldsymbol{\beta}|\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}| :\right\}|\boldsymbol{\epsilon}\rangle\langle\boldsymbol{\epsilon}|$$

$$= \frac{1}{N}\int d\underline{\gamma}d\underline{\beta}d\underline{\alpha}d\underline{\epsilon}\,|\boldsymbol{\gamma}\rangle\langle\boldsymbol{\epsilon}|\exp\left[-(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\mu}+\underline{I}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$

$$\times\left(\frac{\boldsymbol{\beta}}{\boldsymbol{\alpha}}\right)(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\exp\left[\overline{\boldsymbol{\gamma}}\boldsymbol{\beta} + \overline{\boldsymbol{\alpha}}\boldsymbol{\epsilon} - \overline{\boldsymbol{\alpha}}\boldsymbol{\alpha} - \overline{\boldsymbol{\beta}}\boldsymbol{\beta} - \frac{1}{2}\overline{\boldsymbol{\gamma}}\boldsymbol{\gamma} - \frac{1}{2}\overline{\boldsymbol{\epsilon}}\boldsymbol{\epsilon}\right]$$
$$(B44)$$

where we have used the result that the inner product of two coherent states is, from Eq. (A13)

$$\langle\boldsymbol{\beta}|\boldsymbol{\alpha}\rangle \;=\; \exp\left[\overline{\boldsymbol{\beta}}\boldsymbol{\alpha} - \overline{\boldsymbol{\beta}}\boldsymbol{\beta}/2 - \overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}/2\right]\;. \quad (B45)$$

Next, we employ integration by parts [Eq. (A7)] to replace $\left(\dfrac{\boldsymbol{\beta}}{\boldsymbol{\alpha}}\right)$ by variables that appear in the Gaussian form:

$$\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$
$$\times\left[\left(\frac{\boldsymbol{\beta}}{\boldsymbol{\alpha}}\right)\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)\right](\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})$$
$$=\;\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$
$$\times\left[\left(\begin{array}{c}-\partial_{\overline{\boldsymbol{\beta}}}\\ \partial_{\boldsymbol{\alpha}}\end{array}\right)\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)\right](\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})$$
$$\rightarrow\;\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)$$
$$\times\left(\begin{array}{c}\partial_{\overline{\boldsymbol{\beta}}}\\ -\partial_{\boldsymbol{\alpha}}\end{array}\right)\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right](\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})$$
$$=\;\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)\left[\underline{\underline{I}}\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})-\underline{\underline{I}}\right]$$
$$\times\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]\;. \tag{B46}$$

We can now express the result as a derivative of the unnormalised Gaussian operator with respect to $\underline{\underline{\mu}}$:

$$\left\{\widehat{\underline{b}}:\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}:\right\}=\frac{1}{N}\int d\underline{\gamma}d\underline{\beta}d\underline{\alpha}d\underline{\epsilon}\,|\boldsymbol{\gamma}\rangle\langle\boldsymbol{\epsilon}|$$
$$\times\exp\left[-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}-\frac{1}{2}\overline{\boldsymbol{\gamma}}\boldsymbol{\gamma}-\frac{1}{2}\overline{\boldsymbol{\epsilon}}\boldsymbol{\epsilon}+\overline{\boldsymbol{\gamma}}\boldsymbol{\beta}+\overline{\boldsymbol{\alpha}}\boldsymbol{\epsilon}\right]$$
$$\times\left[\underline{\underline{I}}\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\frac{d}{d\underline{\underline{\mu}}}-\underline{\underline{I}}\right]\exp\left[-\frac{1}{2}(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)\right]$$
$$=\frac{1}{N}\left[\underline{\underline{I}}\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\frac{d}{d\underline{\underline{\mu}}}-\underline{\underline{I}}\right]\widehat{\Lambda}^{(u)}\;. \tag{B47}$$

Finally, we can change variables to $\underline{\underline{\sigma}}=[\underline{\underline{\mu}}+2\underline{\underline{I}}]^{-1}$ and use the result for the derivative of the normalisation:

$$\left\{\widehat{\underline{b}}:\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}:\right\}\;=\;\frac{1}{N}\left[-\underline{\underline{I}}\left(\underline{\underline{\sigma}}^{-1}-\underline{\underline{I}}\right)\underline{\underline{\sigma}}\frac{d\widehat{\Lambda}^{(u)}}{d\underline{\underline{\sigma}}}\underline{\underline{\sigma}}-\underline{\underline{I}}\widehat{\Lambda}^{(u)}\right]$$
$$=-\;\underline{\underline{I}}\left(\underline{\underline{\sigma}}^{-1}-\underline{\underline{I}}\right)\underline{\underline{\sigma}}\left(\frac{d\widehat{\Lambda}}{d\underline{\underline{\sigma}}}+\frac{\widehat{\Lambda}}{N}\frac{dN}{d\underline{\underline{\sigma}}}\right)\underline{\underline{\sigma}}-\underline{\underline{I}}\widehat{\Lambda}$$
$$=\;\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\left(\frac{d\widehat{\Lambda}}{d\underline{\underline{\sigma}}}-\widehat{\Lambda}\underline{\underline{\sigma}}^{-1}\right)\underline{\underline{\sigma}}-\underline{\underline{I}}\widehat{\Lambda}$$
$$=\;-\underline{\underline{\sigma}}\widehat{\Lambda}+\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\frac{d\widehat{\Lambda}}{d\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\;. \tag{B48}$$

QED.

7. Antinormal products

Theorem 6: An antinormally ordered product of a pair of ladder operators and a Gaussian is equivalent to a first-order differential operator on the Gaussian, as follows:

$$\left\{\widehat{\underline{b}}\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}\right\}\;=\;\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\widehat{\Lambda}-\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right)\frac{\partial\widehat{\Lambda}}{\partial\underline{\underline{\sigma}}}\left(\underline{\underline{\sigma}}-\underline{\underline{I}}\right) \tag{B49}$$

Proof: The proof initially proceeds in the same manner as for products of mixed ordering. We first insert the coherent state identity to convert the action of the operators into integrals over coherent-state projectors:
$$\left\{\widehat{\underline{b}}\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}\right\}=$$

$$\int d\underline{\gamma}d\underline{\beta}d\underline{\alpha}d\underline{\epsilon}\,|\boldsymbol{\gamma}\rangle\langle\boldsymbol{\gamma}|\left\{\widehat{\underline{b}}\widehat{\underline{b}}^{\dagger}|\boldsymbol{\beta}\rangle\langle\boldsymbol{\beta}|\widehat{\Lambda}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}|\right\}|\boldsymbol{\epsilon}\rangle\langle\boldsymbol{\epsilon}|$$
$$=\frac{1}{N}\int d\underline{\gamma}d\underline{\beta}d\underline{\alpha}d\underline{\epsilon}\,|\boldsymbol{\gamma}\rangle\langle\boldsymbol{\epsilon}|\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$
$$\times\left(\frac{\boldsymbol{\beta}}{\boldsymbol{\alpha}}\right)(\overline{\boldsymbol{\alpha}},\boldsymbol{\beta})\exp\left[\overline{\boldsymbol{\gamma}}\boldsymbol{\beta}+\overline{\boldsymbol{\alpha}}\boldsymbol{\epsilon}-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}-\frac{1}{2}\overline{\boldsymbol{\gamma}}\boldsymbol{\gamma}-\frac{1}{2}\overline{\boldsymbol{\epsilon}}\boldsymbol{\epsilon}\right] \tag{B50}$$

This time, however, we integrate by parts twice:

$$\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$
$$\times\left(\frac{\boldsymbol{\beta}}{\boldsymbol{\alpha}}\right)(\overline{\boldsymbol{\alpha}},\boldsymbol{\beta})\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)$$
$$=\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$
$$\times\left(\begin{array}{c}-\partial_{\overline{\boldsymbol{\beta}}}\\ \partial_{\boldsymbol{\alpha}}\end{array}\right)\left(\partial_{\boldsymbol{\alpha}},-\partial_{\overline{\boldsymbol{\beta}}}\right)\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)$$
$$\rightarrow\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)\left(\begin{array}{c}-\partial_{\overline{\boldsymbol{\beta}}}\\ \partial_{\boldsymbol{\alpha}}\end{array}\right)\left(\partial_{\boldsymbol{\alpha}},-\partial_{\overline{\boldsymbol{\beta}}}\right)$$
$$\times\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right]$$
$$=\exp\left(-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha}-\overline{\boldsymbol{\beta}}\boldsymbol{\beta}\right)\left[-\underline{\underline{I}}+\underline{\underline{I}}\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\right]$$
$$\times\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\underline{\underline{I}}\exp\left[-\,(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha})\left(\underline{\underline{\mu}}+\underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)/2\right] \tag{B51}$$

which is now in a form that we can again express as a derivative of the unnormalised Gaussian operator with

respect to $\underline{\underline{\mu}}$:

$$\left\{\widehat{\underline{b}}\widehat{\underline{b}}^{\dagger}\widehat{\Lambda}\right\} = \frac{-1}{N} \int d\underline{\gamma} d\underline{\beta} d\underline{\alpha} d\underline{\epsilon} \, |\underline{\gamma}\rangle\langle\underline{\epsilon}|$$

$$\times \exp\left[-\overline{\boldsymbol{\alpha}}\boldsymbol{\alpha} - \frac{1}{2}\overline{\boldsymbol{\beta}}\boldsymbol{\beta} - \overline{\boldsymbol{\gamma}}\boldsymbol{\gamma} - \frac{1}{2}\overline{\boldsymbol{\epsilon}}\boldsymbol{\epsilon} + \overline{\boldsymbol{\gamma}}\boldsymbol{\beta} + \overline{\boldsymbol{\alpha}}\boldsymbol{\epsilon}\right]$$

$$\times \left(\left[\underline{\underline{I}} - \underline{\underline{I}}\left(\underline{\underline{\mu}} + \underline{\underline{I}}\right)\frac{d}{d\underline{\underline{\mu}}}\right] \exp\left[-\frac{1}{2}\left(\overline{\boldsymbol{\beta}},\boldsymbol{\alpha}\right)\left(\underline{\underline{\mu}} + \underline{\underline{I}}\right)\left(\frac{\boldsymbol{\alpha}}{\boldsymbol{\beta}}\right)\right]\right)$$

$$\times \left(\underline{\underline{\mu}} + \underline{\underline{I}}\right)\underline{\underline{I}}$$

$$= \frac{1}{N}\left[-\underline{\underline{I}}\widehat{\Lambda}^{(u)} + \underline{\underline{I}}\left(\underline{\underline{\mu}} + \underline{\underline{I}}\right)\frac{d\widehat{\Lambda}^{(u)}}{d\underline{\underline{\mu}}}\right]\left(\underline{\underline{\mu}} + \underline{\underline{I}}\right)\underline{\underline{I}} \ . \qquad \text{(B52)}$$

Finally, we change variables to $\underline{\underline{\sigma}} = [\underline{\underline{\mu}} + 2\underline{\underline{I}}]^{-1}$ and use the result for the derivative of the normalisation:

$$\left\{\widehat{\underline{b}}\widehat{\underline{b}}^{\dagger}\widehat{\Lambda} :\right\} = \frac{1}{N}\left[\underline{\underline{I}}\widehat{\Lambda}^{(u)} - \underline{\underline{I}}\left(\underline{\underline{I}} - \underline{\underline{\sigma}}^{-1}\right)\underline{\underline{\sigma}}\frac{d\widehat{\Lambda}^{(u)}}{d\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]\left(\underline{\underline{I}} - \underline{\underline{\sigma}}^{-1}\right)\underline{\underline{I}}$$

$$= \left(\underline{\underline{\sigma}} - \underline{\underline{I}}\right)\widehat{\Lambda} - \left(\underline{\underline{\sigma}} - \underline{\underline{I}}\right)\frac{d\widehat{\Lambda}}{d\underline{\underline{\sigma}}}\left(\underline{\underline{\sigma}} - \underline{\underline{I}}\right) \ . \qquad \text{(B53)}$$

QED.

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